

SYMMETRY AND DIRAC POINTS IN GRAPHENE SPECTRUM

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ABSTRACT. Existence and stability of Dirac points in the dispersion relation of operators periodic with respect to the hexagonal lattice is investigated for different sets of additional symmetries. The following symmetries are considered: rotation by $2\pi/3$ and inversion, rotation by $2\pi/3$ and horizontal reflection, inversion or reflection with weakly broken rotation symmetry, and the case where no Dirac points arise: rotation by $2\pi/3$ and vertical reflection.

All proofs are based on symmetry considerations and are elementary in nature. In particular, existence of degeneracies in the spectrum is proved by a transplantation argument (which is deduced from the (co)representation of the relevant symmetry group). The conical shape of the dispersion relation is obtained from its invariance under rotation by $2\pi/3$. Persistence of conical points when the rotation symmetry is weakly broken is proved using a geometric phase in one case and parity of the eigenfunctions in the other.

1. INTRODUCTION

Many interesting physical properties of graphene are consequences of existence of special points in its dispersion relation [28, 8, 21, 13]. These points, sometimes referred to as Dirac points, are conical singularities, where two sheets of the dispersion relation touch at a point and are linear in any outward direction.

Most mathematical analysis of the dispersion relation of graphene is performed in physics literature in the tight-binding approximation, starting from the work of Wallace [37] and Slonczewski and Weiss [34]. This is equivalent to modeling the material as a discrete graph with vertices at the carbon molecules' locations and with edges indicating chemical bonds. A richer mathematical model for graphene was considered by Kuchment and Post in [23], who studied quantum graphs with potential on edges, arranged to form a honeycomb lattice.

The \mathbb{R}^2 Schrödinger operator $H_\varepsilon = -\Delta + \varepsilon q(\vec{x})$ with the real-valued potential $q(\vec{x})$ that has honeycomb symmetry was considered by Grushin [17]. A condition for a multiple eigenvalue to be a conical point was established and checked in the perturbative regime of a weak potential (small ε). The multiplicity of the eigenvalue was proved from the symmetry point of view, an approach that we fully develop here.

The case of potential of arbitrary strength was studied by Fefferman and Weinstein [12]. Their results can be schematically broken into three parts: (a) establish that the dispersion relation has a double degeneracy at certain known values of quasi-momenta; (b) establish that for almost all ε the dispersion relation is conical in the vicinity of the degeneracy; (c) prove that the conical singularities survive under weak perturbation destroying some of the symmetries of the potential (namely, the rotational symmetry). These results are contained in [12, Thms 5.1(1), 4.1 and 9.1] with proofs which are rather technical.

The purpose of this article is to make explicit the role of symmetry in existence and stability of Dirac points and to give proofs that are at the same time simpler and more general. Our methods apply to many different settings: graphs (discrete or quantum), Schrödinger and Dirac operators on \mathbb{R}^2 . We use Schrödinger operator as our primary focus, and give numerical examples using discrete graphs. We also consider the effect of different symmetries, substituting inversion symmetry, usually assumed in the literature, with horizontal reflection symmetry (the results are analogous or stronger, as explained below).

We will now briefly review our results and the methods employed. The Schrödinger operator is assumed to be shift-invariant with respect to the hexagonal lattice. We also consider the following symmetries (see Fig. 1 for an illustration): rotation by $2\pi/3$ (henceforth, “rotation”), inversion (reflection with respect to the point $(0,0)$), horizontal reflection and, to a lesser extent, vertical reflection. We remark that horizontal and vertical reflections are substantially different because the hexagonal lattice is not invariant with respect to rotation by $\pi/2$. We study the question of existence of Dirac points when the operator has various subsets of the above symmetries.

We show that existence of the degeneracy is a direct consequence of symmetries of the operator. The natural tool for studying this is, of course, the representation theory. It is well known that existence of a two- (or higher) dimensional irreducible representation suggests that some eigenvalues will be degenerate. However, rotation combined with inversion — the most usual choice of symmetries [17, 12] — is an abelian group, whose irreps are all one-dimensional. The resolution of this question lies in the fact that the relevant symmetry is the inversion combined with complex conjugation and one should look at representations combining unitary and antiunitary operators, the so-called *corepresentations* introduced and fully classified by Wigner [41, Chap. 26].

To prove the existence of the degeneracy in the spectrum (Theorem 4.1) we split the operator into three parts and use the “transplantation proof” to prove isospectrality of two parts. The representation theory (in particular, checking the isospectrality condition of Band–Parzanchevski–Ben-Shach [4, 30]) is kept behind the scenes, in Appendix B. There are three reasons for this. First, the transplantation proof is extremely simple and short, it requires no knowledge of representation theory and can be read immediately after the dispersion relation is defined in section 1.3. Second, the same proof works for the two cases where we establish a positive result: rotation coupled with inversion and rotation coupled with horizontal reflection. Third, to show that a two-dimensional representation leads to doubly-degenerate eigenvalue one has to show that the corresponding isotypic component of the Hilbert space is non-empty, which requires work. The transplantation proof hides that work under the hood too.

The conical nature of the dispersion relation is known to be a generic situation (see, for example, [1, Appendix 10]); to prove it in a particular case one uses perturbation theory, as done in [17] and, implicitly, in [12]. Again, we seek to make the effect of symmetry most explicit here. This is done on two levels. First, in Corollary 3.2 and Lemma 3.4 we show that the dispersion relation also has rotational symmetry and thus, by Hilbert-Weyl theory of invariant functions, is restricted to be a circular cone (which could be degenerate) plus higher order terms. Then, in Theorem 5.2, we show that the symmetries also enforce a certain relation on the first order terms of the perturbative expansion of the operator, which restricts the possible form of the terms. In spirit, this conclusion parallels the Hilbert-Weyl theory, but is somewhat more powerful: it further allows us to conclude that at quasimomentum $\vec{0}$, where we discover persistent degeneracies with only the rotational symmetry, the dispersion relation is locally flat.

Part (c) of the above classification, the survival of the Dirac points when a weak perturbation breaks the rotational symmetry, can be established by perturbation theory, as done in [12]. However, such resilience of singularities indicates that there are topological obstacles to their disappearance [26, 25, 27]. The method familiar to physicists is to use the Berry phase [5, 33], which works when the operator has inversion symmetry (Section 7.1). Interestingly, when instead of inversion symmetry we have horizontal reflection symmetry, Berry phase is *not* restricted to the integer multiples of π and the topological obstacle has a different nature. The survival of the Dirac cone is shown to be a consequence of the structure of representation of the reflection symmetry (Section 7.2), which combines eigenfunctions of different parities at the degeneracy point. As a consequence of our proof we conclude that the perturbed cone, although shifted from the corner of the Brillouin zone, remains on a certain explicitly defined line. In particular, this restricts the location of points in the Brillouin zone where Dirac cones can be destroyed by merging with their symmetric counterparts. Naturally, this effect is also present when there is horizontal reflection symmetry *in addition* to the

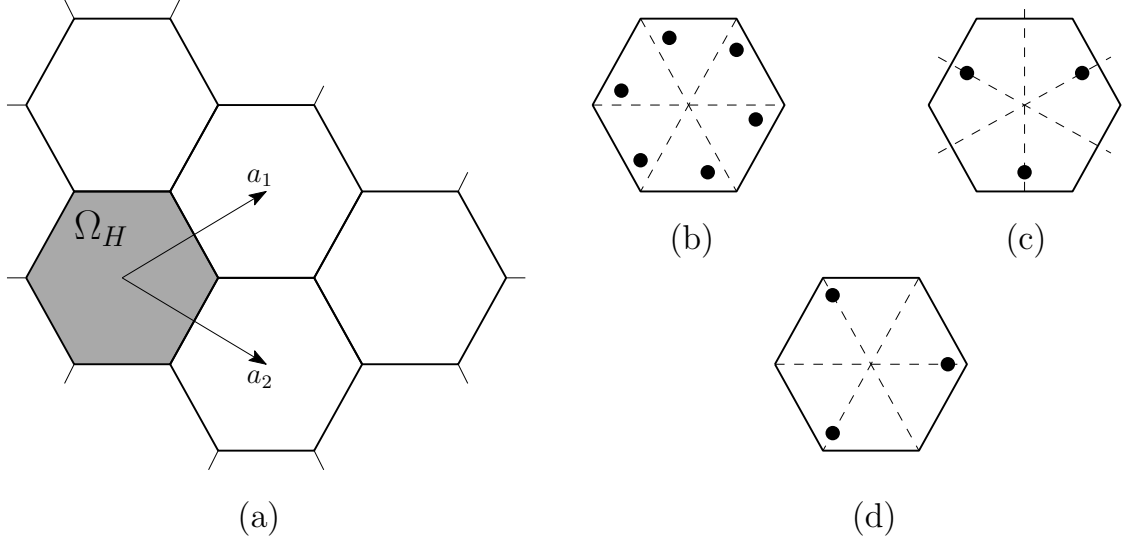


FIGURE 1. Hexagonal lattice (a) and examples of fundamental domains with symmetry R and, additionally, (b) inversion symmetry V , (c) horizontal reflection symmetry F and (d) vertical reflection symmetry F_V . Note that we do not expect conical points in operators with symmetries R and F_V , see section B.3.

inversion symmetry. We remark that experimentally created potentials usually possess the reflection symmetry, [3, 36].

To summarize, in addition to providing simpler and shorter symmetry-based proofs to existing results, we discover some previously unknown consequences. In particular, we consider the case of rotational symmetry coupled with horizontal reflection symmetry; in this case when the rotational symmetry is weakly destroyed, the conical points travel on a special line. We observe degeneracies at quasimomentum $\vec{0}$ in presence of rotational symmetry only; the dispersion relation at this point is shown to be locally flat. Finally, we explain why the coupling of rotation and vertical reflection *does not*, in general, lead to the appearance of Dirac points. The tools developed in this article would be easily extensible to other lattice structures [9] and graphene superlattices [42, 31].

1.1. Symmetries. The periodicity lattice of the operators we will consider is the 2-dimensional hexagonal lattice Γ with the basis vectors

$$(1) \quad \vec{a}_1 = \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \end{pmatrix}, \quad \vec{a}_2 = \begin{pmatrix} \sqrt{3}/2 \\ -1/2 \end{pmatrix},$$

see Fig. 1(a). The operator considered will always be assumed to be invariant with respect to the shifts by this lattice.

In addition to the shifts, the lattice Γ has several other symmetries. We now describe some of them as operators acting on functions on \mathbb{R}^2 (or on a graph embedded into \mathbb{R}^2).

- Rotation R by $2\pi/3$ in the positive (counter-clockwise) direction:

$$R : \psi(x_1, x_2) \mapsto \psi \left(-\frac{1}{2}x_1 + \frac{\sqrt{3}}{2}x_2, -\frac{\sqrt{3}}{2}x_1 - \frac{1}{2}x_2 \right).$$

- Inversion V :

$$V : \psi(x_1, x_2) \mapsto \psi(-x_1, -x_2).$$

- Horizontal reflection F :

$$F : \psi(x_1, x_2) \mapsto \psi(-x_1, x_2).$$

Note that R and V together form the abelian group of rotations by multiples of $\pi/3$; VF is the vertical reflection. In what follows, we will assume our operator has symmetries generated by a subset of the R , V and F .

As the base operator (i.e. before we apply Floquet-Bloch analysis) we will always take an operator with real coefficients, thus it will be symmetric with respect to complex conjugation. As it turns out, an important role is played by the product of inversion and complex conjugation,

- Symmetry \bar{V} :

$$\bar{V} : \psi(x_1, x_2) \mapsto \overline{\psi(-x_1, -x_2)}.$$

Note that \bar{V} is not a \mathbb{C} -linear operator; it is, however, a linear operator over reals.

Finally, we will also consider the vertical reflection symmetry:

- Vertical reflection F_V :

$$F_V : \psi(x_1, x_2) \mapsto \psi(x_1, -x_2).$$

Its effect is not the same as that of the horizontal reflection F because the two symmetries are aligned differently with respect to the lattice Γ . In fact, in contrast to F , the presence of F_V (in addition to symmetry R) does not generally lead to the appearance of conical points in the dispersion relation. This negative result is also important to understand; we explain it in section B.3.

In Fig. 1(b-d) we show the fundamental domain of the lattice with defects that have symmetry R in addition to V , F or F_V , correspondingly.

1.2. Operators. As our primary motivational example we use the two-dimensional Schrödinger operator

$$(2) \quad H = -\Delta + q(\vec{x})$$

with the real-valued potential $q(\vec{x})$ assumed to be smooth and periodic with respect to the lattice Γ . For general properties of the dispersion relation of such operators we refer the reader to [2, 22].

To generate simple numerical examples we use discrete Schrödinger operators with potentials crafted to break or retain some of symmetries listed above. More precisely, denote by $G = (V, E)$ an infinite graph embedded in \mathbb{R}^2 , with vertex set V and edge set E . The embedding is realized by the mapping $\text{loc} : V \rightarrow \mathbb{R}^2$ which gives the location in \mathbb{R}^2 of the given vertex. A transformation $T : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ preserves the graph structure if $u_1, u_2 \in V$ implies existence of $u'_1, u'_2 \in V$ such that $T \text{loc}(u_j) = \text{loc}(u'_j)$ and u'_1, u'_2 are connected by an edge if and only if u_1, u_2 are connected.

The graph is Λ -periodic if the graph structure is preserved by the shifts defining the lattice. A graph with space symmetry S is defined analogously.

The Schrödinger operator is defined on the functions from $\ell^2(\mathbb{C}^V)$ by

$$(3) \quad (Hf)_v = \sum_{(v,u) \in E} m_{v,u}(f_v - f_u) + q_v f_v,$$

where the sum is over all vertices u adjacent to v , $m_{v,u} > 0$ are weights associated to edges (often, they are taken inversely proportional to edge length) and $q : V \rightarrow \mathbb{R}$ is the discrete potential. In our examples, the graph structure will be compatible with all symmetries of the lattice Λ , while m and q will be breaking some of the point symmetries (however, they will always be periodic). The simplest Γ -periodic graph is shown in Fig. 9(a). This is the graph arising as the tight-binding approximation of graphene.

Note that the discrete Schrödinger operator of graphs with more than two atoms per unit cell is not a mere mathematical curiosity since it arises in studying the twisted graphene and graphene in a periodic potential (superlattice), see [24, 42, 38] and references therein.

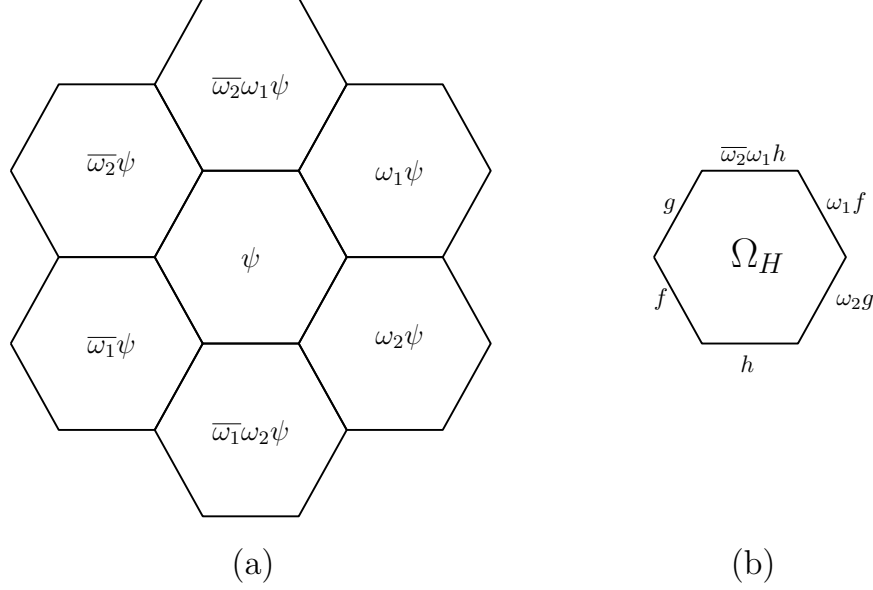


FIGURE 2. Floquet-Bloch reduction on the plane with hexagonal lattice generated by \vec{a}_1 and \vec{a}_2 .

1.3. Floquet-Bloch reduction. Floquet theory can be thought of as a version of Fourier expansion, mapping the spectral problem on a non-compact manifold into a continuous sum of spectral problems on a compact manifold. The compact spectral problems are parametrized by the representations of the abelian group of periods (shifts).

Denote by $\mathcal{X}(\vec{k})$, $\vec{k} = (k_1, k_2) \in \mathbb{T}^2 := [0, 2\pi)^2$ the space of Bloch functions, i.e. locally L^2 functions satisfying

$$(4) \quad \psi(\vec{x} + n_1\vec{a}_1 + n_2\vec{a}_2) = e^{i(n_1k_1 + n_2k_2)}\psi(x), \quad n_1, n_2 \in \mathbb{Z}.$$

For $\psi \in \mathcal{X}(\vec{k})$ which also belong to the domain of H it can be immediately seen that

$$(H\psi)(x + n_1\vec{a}_1 + n_2\vec{a}_2) = e^{i(n_1k_1 + n_2k_2)}H\psi(x),$$

i.e. the space $\mathcal{X}(\vec{k})$ is invariant under H . By $H(\vec{k})$ we will denote the restriction of the operator H to the space $\mathcal{X}(\vec{k})$. Its domain is $\mathcal{X}^2(\vec{k})$, the dense subspace of $\mathcal{X}(\vec{k})$ consisting of functions that locally belong to L^2 together with their derivatives up to the second order.

Choosing a fundamental domain¹ of the action of the group of periods, we can reduce the problem to the fundamental domain with quasi-periodic boundary conditions.

The result of the Floquet-Bloch reduction is shown in Fig. 2. In Fig. 1(a), the lattice generating vectors \vec{a}_1 and \vec{a}_2 were shown together with a convenient choice of the fundamental region (shaded) and its four translations, by \vec{a}_1 , \vec{a}_2 , $\vec{a}_1 - \vec{a}_2$ and $\vec{a}_1 + \vec{a}_2$. This choice of the fundamental domain we will be denoting by Ω_H . The values of a Bloch function in surrounding regions, according to equation (4), are indicated in Fig. 2(a), using the notation

$$(5) \quad \omega_j = e^{ik_j}, \quad j = 1, 2.$$

The continuity of the function and its derivative across the boundaries of copies of the fundamental region impose boundary conditions shown schematically in Fig. 2(b). They should be understood

¹a domain having the property that each trajectory $\{\vec{x} + n_1\vec{a}_1 + n_2\vec{a}_2 : n_1, n_2 \in \mathbb{Z}\}$ has exactly one representative in it

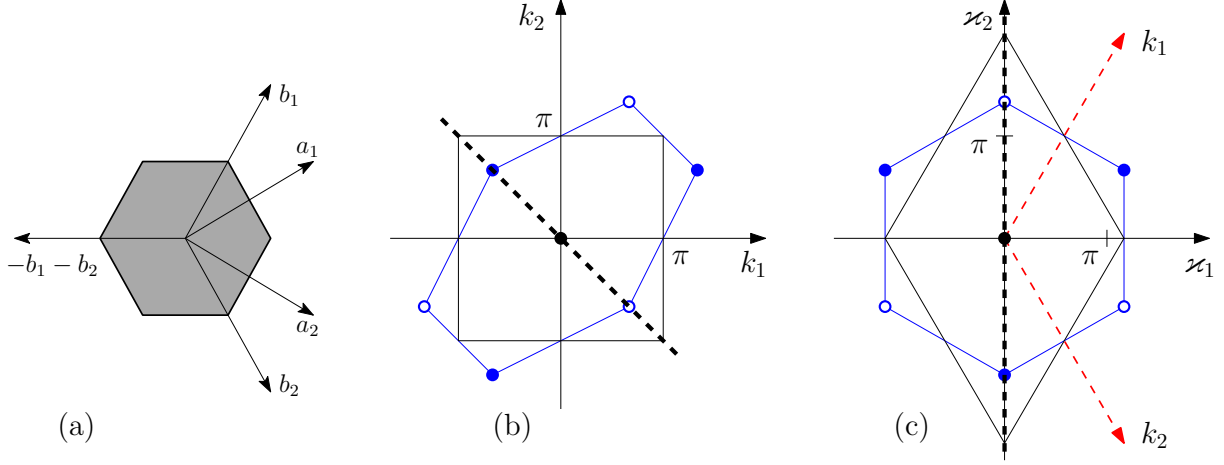


FIGURE 3. The dual basis (a) to the vectors \vec{a}_1 and \vec{a}_2 and two choices of the Brillouin zone in terms of (b) coordinates k_1, k_2 (drawn as if they are Cartesian) and (c) coordinates κ_1, κ_2 (which are Cartesian); part (c) also shows the correct position for the axes k_1 and k_2 . The axis of symmetry of the operator \hat{F} is shown in dashed line (equation $k_1 = -k_2$). Fixed points of the operator \hat{R} are shown by circles (different fill styles correspond to different points of symmetry).

as follows: taking the bottom and top boundaries as an example, and parametrizing them left to right, the conditions read

$$\psi|_{\text{top}} = \bar{\omega}_2 \omega_1 \psi|_{\text{bottom}}, \quad -\partial_{\vec{n}} \psi|_{\text{top}} = \bar{\omega}_2 \omega_1 \partial_{\vec{n}} \psi|_{\text{bottom}},$$

where the normal derivative is taken in the outward direction (this causes the minus sign to appear). We stress again that in Fig. 2(c) we use letters f, g and h as placeholder labels, connecting the values of the function and its derivative on similarly labeled sides.

To represent the exponent of the Bloch phase $n_1 k_1 + n_2 k_2$ as a scalar product, we introduce the vectors

$$(6) \quad \vec{b}_1 = \left(\frac{1}{\sqrt{3}}, 1 \right)^T, \quad \vec{b}_2 = \left(\frac{1}{\sqrt{3}}, -1 \right)^T,$$

see Fig. 3(a). Then

$$(7) \quad \vec{b}_i^T \cdot \vec{a}_j = \delta_{i,j}.$$

The vectors \vec{b}_1, \vec{b}_2 define a lattice which is known as the *dual lattice*. For a hexagonal lattice, the dual lattice is also hexagonal.

Due to (7), one can write $n_1 k_1 + n_2 k_2$ as the dot product of the vector of the shift $n_1 \vec{a}_1 + n_2 \vec{a}_2$ the vector which has $k_j, j = 1, 2$, as components:

$$n_1 k_1 + n_2 k_2 = (k_1 \vec{b}_1 + k_2 \vec{b}_2) \cdot (n_1 \vec{a}_1 + n_2 \vec{a}_2).$$

Let us comment on using coordinates k_1, k_2 which are the coordinates with respect to the basis \vec{b}_1, \vec{b}_2 versus the corresponding Cartesian coordinates κ_1, κ_2 given by

$$(8) \quad \vec{\kappa} = \begin{pmatrix} 1/\sqrt{3} & 1/\sqrt{3} \\ 1 & -1 \end{pmatrix} \vec{k} =: B \vec{k}.$$

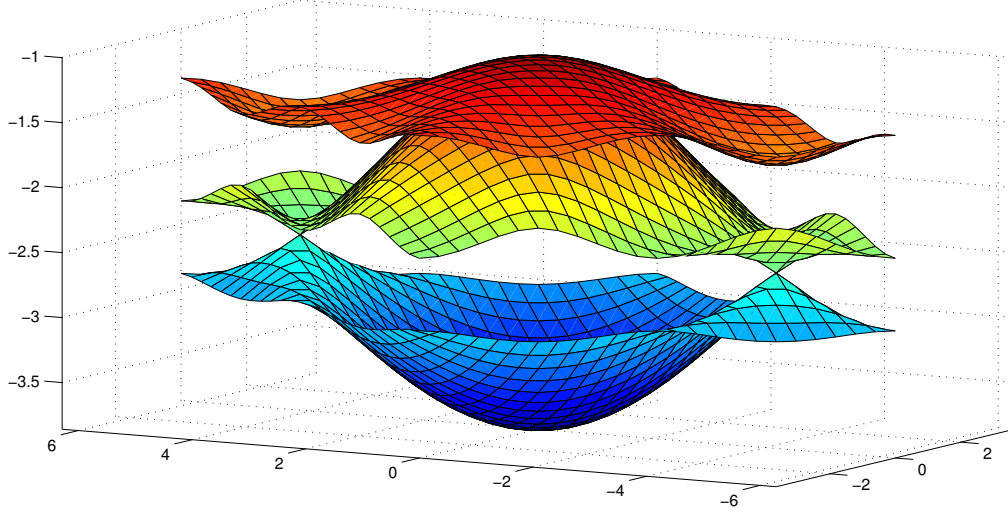


FIGURE 4. The lowest three bands of the dispersion relation of the graph from Example 4.4, which has reflection symmetry. The lower two bands touch conically at the points $\pm \vec{k}^*$. The Brillouin zone is parametrized by \vec{x} coordinates.

In Fig. 3(b) we show two choices of the Brillouin zone² drawn in terms of coordinates k_1, k_2 and coordinates κ_1, κ_2 . The first picture one gets if one uses k_1 and k_2 as parameters for the dispersion relation (which is natural) ranging from $-\pi$ to π (black square) and then plots the result using k_1 and k_2 as Cartesian coordinates. The resulting plot of the dispersion relation will be skewed similarly to the blue hexagon in Fig. 3(b) (cf. Figures 5 and 6 of [23]). A more correct way of plotting is over a domain in Fig. 3(c), as it will highlight the symmetries of the result (see Figs. 4 and 5 and the explanations in the following section).

2. FORMULATION OF RESULTS

For each value of the quasi-momentum \vec{k} , the operator $H(k)$ has discrete spectrum. Its eigenvalues as functions of \vec{k} is what is known as the *dispersion relation*. Our results are concerned with the structure of the dispersion relation for the operators we described in Section 1.2. A typical example is shown in Fig. 4; it was computed for a discrete Laplacian described in detail in Example 4.4.

In the figure, one can see two *conical points* where the lowest two sheets of the dispersion relation touch. In terms of \vec{k} coordinates, they touch at $\pm \vec{k}^*$, where

$$\vec{k}^* = \left(\frac{2\pi}{3}, -\frac{2\pi}{3} \right).$$

The second and third sheets also touch, at the point $\vec{0} = (0, 0)$; at the point of contact both surfaces are locally flat. We will show that these features are typical: conical singularities at the point \vec{k}^* and flat contact at the point $\vec{0}$.

Theorem 2.1. *Let the self-adjoint operator with real coefficients H be invariant under the shifts by lattice Γ , rotation R and at least one of the following: reflection F or inversion V . Let \vec{k}_0 be one of the points \vec{k}^* , $-\vec{k}^*$ or $\vec{0}$. Then*

- (1) *The operator $H(\vec{k}_0)$ splits into a direct sum of three self-adjoint operators (which are different at $\pm \vec{k}^*$ and $\vec{0}$),*

$$H(\vec{k}_0) = Q_0 \oplus Q_1 \oplus Q_2.$$

²By “Brillouin zone” we understand *any* choice of the fundamental domain of the dual lattice. What is known as the “first Brillouin zone” is the hexagonal domain in blue in Fig. 3(c)

(2) *The operators Q_1 and Q_2 are isospectral. Therefore, $H(\vec{k}_0)$ has some eigenvalues with multiplicity at least 2.*

(3) *If the multiplicity of an eigenvalue $\lambda_0 \in \sigma(H(\vec{k}_0))$ is exactly 2, the dispersion relation in coordinates \vec{x} is given by*

$$(9) \quad (\lambda - \lambda_0)^2 = |\alpha|^2 |\vec{x} - \vec{x}_0|^2 + o(|\vec{x} - \vec{x}_0|^2).$$

(4) *At the point $\vec{k}_0 = \vec{0}$ the coefficient $|\alpha|$ is zero.*

Note that we will give an explicit definition of the operators Q_j as operators on a subdomain of Ω_H with some special boundary conditions.

By Theorem 2.1, we are guaranteed to have conical points (i.e. points where the dispersion relation is of the form (9)) whenever two conditions are satisfied: an eigenvalue of Q_1 is simple and is not in the spectrum of Q_0 , and the parameter $\alpha \neq 0$. Intuitively, it is clear that both conditions are “generic”: if either of them is broken, any typical small perturbation of the potential should restore it.

To make this intuition precise, we consider the operator $H = -\Delta + \varepsilon q(\vec{x})$, where we are able to say more about the parameter α and the exact multiplicity of eigenvalues.

Theorem 2.2. *Let $H = -\Delta + \varepsilon q(\vec{x})$ with bounded measurable real potential $q(\vec{x})$ which is invariant under the shifts by lattice Γ , rotation R and at least one of the following: reflection F or inversion V . Further, assume that condition*

$$(10) \quad \int_{\Omega_H} e^{\frac{4\pi i}{\sqrt{3}}x_1} q(\vec{x}) d\vec{x} \neq 0,$$

is satisfied. Then the following conditions break on at most a discrete set of $\varepsilon \in \mathbb{R}$:

- (1) *there is an eigenvalue $\lambda_0(\varepsilon)$ of Q_1 which is simple and which is the smallest eigenvalue of Q_1 for small ε ,*
- (2) *the eigenvalue $\lambda_0(\varepsilon) \notin \sigma(Q_0)$,*
- (3) *the corresponding α in equation (9) is non-zero.*

We mention that condition (10) above is equivalent to condition (5.2) of [12] when one takes into account symmetries (such as (2.36) of [12]).

We now consider the fate of a conical point when the rotational symmetry is broken by a small perturbation.

Theorem 2.3. *Let H be an operator satisfying the conditions of Theorem 2.1. Assume its dispersion relation has a nondegenerate conical point at the point $\vec{k}_0 = \pm \vec{k}^*$. Consider the perturbed operator $H_\varepsilon := H + \varepsilon W$, where the relatively bounded perturbation W has the same symmetries as H (namely, Γ -invariance and \bar{V} - or F -invariance) except the R -invariance.*

Then, for small ε , the dispersion relation of H_ε has a nondegenerate conical point in the neighborhood of \vec{k}_0 . Furthermore, if H_ε is invariant with respect to reflection F , the conical point remains on the line $k_2 = -k_1$ modulo 2π .

3. SYMMETRIES OF THE REDUCED OPERATOR

As mentioned before, the operator $H(\vec{k})$ is the restriction of the operator H to the space $\mathcal{X}(\vec{k})$. Equivalently, it can be considered as the operator on the compact domain of Fig. 2(c) with the specified boundary conditions³. It is immediate from the definition of $H(\vec{k})$ that the dispersion relation is invariant with respect to shifts by 2π ,

$$(11) \quad \vec{k} \mapsto \vec{k} + (2\pi, 0) \quad \text{and} \quad \vec{k} \mapsto \vec{k} + (0, 2\pi).$$

³if the operator H is specified on discrete graphs, the “boundary conditions” require special interpretation, see Section 4.1 for some examples

In other words, the dispersion relation is periodic with respect to the dual lattice. We will now study other symmetries of the dispersion relation.

For given values of k_1, k_2 (or, equivalently, ω_1, ω_2), the operator $H(\vec{k})$ may no longer have all the symmetries of the original operator H : while the differential expression defining the operator is still invariant, the domain of definition has been restricted and may not be invariant anymore.

We start with the rotation operator R . We first need to understand the effect of R on the space $\mathcal{X}(\vec{k})$. This can be understood by rotating the picture in Fig. 2(b) by $2\pi/3$ and finding the “new ω_1, ω_2 ”:

$$\omega'_1 = \overline{\omega_1}\omega_2, \quad \omega'_2 = \overline{\omega_1}, \quad \overline{\omega'_2}\omega'_1 = \omega_2.$$

The last equation clearly follows from the first two. For the exponents k'_1, k'_2 , defined as in (5), we have

$$(12) \quad \begin{pmatrix} k'_1 \\ k'_2 \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} =: \hat{R} \begin{pmatrix} k_1 \\ k_2 \end{pmatrix}.$$

With respect to the dual basis \vec{b}_1, \vec{b}_2 , the matrix \hat{R} is unitary; it is the rotation of coordinates by $2\pi/3$, see Fig. 3(a) (and Appendix A for further discussion).

Since the operator $H(\vec{k})$ is the restriction of the operator H , which is invariant under the rotation R , to the space $\mathcal{X}(\vec{k})$, we get

Lemma 3.1. *R acts as a unitary operator from $\mathcal{X}(\vec{k})$ to $\mathcal{X}(\hat{R}\vec{k})$. Therefore,*

$$(13) \quad H(\vec{k}) = R^* H(\hat{R}\vec{k}) R.$$

As a consequence, each sheet $\lambda_n(\vec{k})$ of the dispersion relation is invariant under the mapping

$$(14) \quad \vec{k} \mapsto \hat{R}\vec{k} \mod 2\pi\mathbb{Z}^2,$$

which maps a Brillouin zone to itself. The fixed points of this mapping are the points

$$(15) \quad \vec{k}^* := (2\pi/3, -2\pi/3), \quad -\vec{k}^* := (-2\pi/3, 2\pi/3), \quad \vec{0} := (0, 0),$$

and their shifts by 2π . In coordinates \varkappa , the mapping acts as a rotation by $2\pi/3$ around each of the fixed points

$$(16) \quad \vec{\varkappa}^* := (0, 4\pi/3), \quad -\vec{\varkappa}^* := (0, -4\pi/3), \quad \vec{0} := (0, 0),$$

Proof. Equation (13) follows immediately from R being a symmetry of H (i.e. $H = R^* H R$) and H leaving spaces $\mathcal{X}(\vec{k})$ to $\mathcal{X}(\hat{R}\vec{k})$ invariant.

From (13), we immediately conclude that the spectra of $H(\vec{k})$ and $H(\hat{R}\vec{k})$ are the same, i.e. the dispersion relation is invariant under the rotation \hat{R} . The invariance under the shift by 2π in either coordinate was already explained above. The rest is a simple calculation. \square

Analogous considerations for the horizontal reflection F result in

$$\omega'_1 = \overline{\omega_2}, \quad \omega'_2 = \overline{\omega_1},$$

and, eventually, in

$$(17) \quad FH(\vec{k})F^* = H(\hat{F}\vec{k}), \quad \text{where} \quad \hat{F} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}.$$

The matrix \hat{F} is a reflection with respect to the line $k_2 = -k_1$ and it leaves the points of this line invariant.

Both complex conjugation and inversion result in

$$\omega'_1 = \overline{\omega_1}, \quad \omega'_2 = \overline{\omega_2},$$

and possess a unique fixed point $\vec{k} = \vec{0}$. However, their composition \overline{V} preserves the boundary conditions for all values of ω_1, ω_2 .

To be more precise, denoting by C the antiunitary operation of taking complex conjugation (or “time-reversal” in physics terminology), we have

$$(18) \quad CH(\vec{k})C^{-1} = H(-\vec{k}) = VH(\vec{k})V^*.$$

Equations (13), (17) and (18) show that the symmetries of the operator result in the symmetries of the dispersion relation. Those are more conveniently stated in $\vec{\varkappa}$ coordinates. We summarize these symmetries for the choices of H that we will study in this paper.

Corollary 3.2. *The dispersion relation of the Γ -periodic operator H is invariant with respect to the dual lattice, i.e. the shifts*

$$(19) \quad \vec{\varkappa} \mapsto \vec{\varkappa} + 2\pi b_1 \quad \text{and} \quad \vec{\varkappa} \mapsto \vec{\varkappa} + 2\pi b_2.$$

If the operator H is invariant with respect to rotation R and time-reversal C , the dispersion relation $\lambda_n(\vec{\varkappa})$ is symmetric with respect to

- *rotation by $\pi/3$ around the point $\vec{0} = (0, 0)$.*
- *rotation by $2\pi/3$ around the points $\pm\vec{\varkappa}^* = \pm(0, 4\pi/3)$.*

If, additionally, the operator has reflection symmetry F , then the symmetry groups increase to

- *D_6 around the point $\vec{0}$,*
- *D_3 around the points $\pm\vec{\varkappa}^*$.*

Above, D_3 and D_6 are the groups of symmetries of equilateral triangle and hexagon.

Remark 3.3. When H is invariant with respect to complex conjugation, inversion symmetry of the operator does not result in any additional symmetries of the dispersion relation.

Proof. Equation (19) is simply equation (11) written in \varkappa coordinates.

From equations (13), (17) and (18) we know that the operator $H(\vec{\varkappa})$ is unitarily equivalent to $H(\hat{S}\vec{\varkappa})$, where S is the appropriate symmetry transformation. In Appendix A the operators \hat{R} and \hat{F} are calculated in $\vec{\varkappa}$ coordinates.

Naturally, \hat{R} is just the rotation by $2\pi/3$ around the origin. Together with the involution $\varkappa \mapsto -\varkappa$ (i.e. rotation by π) induced by the time-reversal symmetry, this makes dispersion relation invariant with respect to rotation by $\pi/3$.

Rotation by $2\pi/3$ followed by the shift by $2\pi b_1$ is equivalent to the rotation by $2\pi/3$ around the point $\varkappa^* = (0, 4\pi/3)$. Similar conclusion applies to the point $-\varkappa^*$. Of course, the points $\pm\varkappa^*$ are simply the points $\pm\vec{\varkappa}^*$ expressed in $\vec{\varkappa}$ coordinates.

Finally, reflection symmetry of the operator adds reflection symmetry to the dispersion relation resulting in the dihedral groups. \square

Figure 5 illustrates the results of Corollary 3.2. Here the contour plots of the two lowest bands of the dispersion relation are shown for the operator H which has the reflection symmetry F in addition to the (usual) rotational and time-reversal symmetries. The contours have symmetries D_3 and D_6 around the fixed points $\pm\vec{\varkappa}^*$ and $\vec{0}$, respectively. Close to the fixed points, the contours became circular. This is also a generic behavior explained in the next lemma.

An important consequence of symmetry is a restriction on the possible local form of the dispersion relation. In particular, the dispersion relation must be a circular cone (which could be degenerate) around a point of multiplicity two.

Lemma 3.4. *Let $\vec{\varkappa}_0$ be one of the symmetry points, $\vec{0}$ or $\pm\vec{\varkappa}^*$.*

(1) *If $\lambda_n(\vec{\varkappa}_0) =: \lambda_0$ is a simple eigenvalue, the dispersion relation is given locally by*

$$(20) \quad \lambda - \lambda_0 = a|\vec{\varkappa} - \vec{\varkappa}_0|^2 + o(|\vec{\varkappa} - \vec{\varkappa}_0|^2), \quad a \in \mathbb{R}.$$

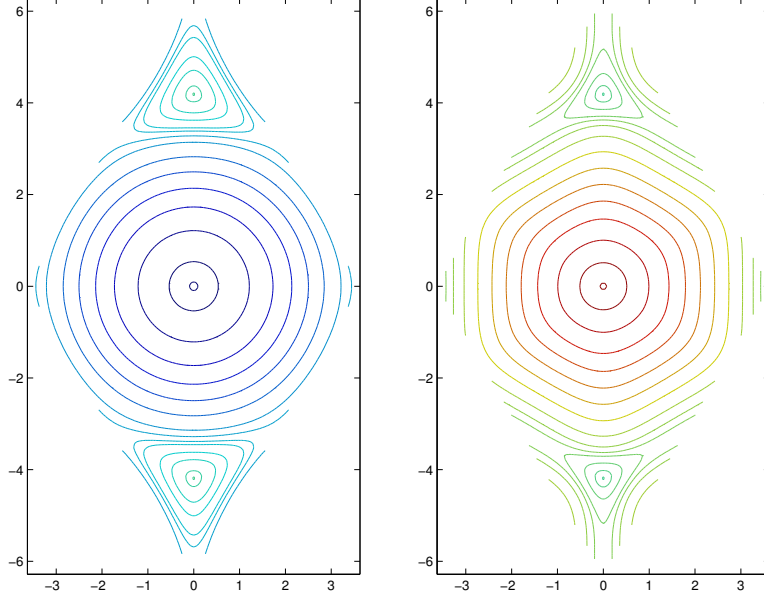


FIGURE 5. The contour plots of the two lowest bands from Fig. 4. Because of rotational symmetry, the contours are symmetric under the rotation by $2\pi/3$ around the points $(0,0)$ and $\pm\vec{z}^*$. In addition, the operator has reflection symmetry and the plots are symmetric with respect to the vertical axis.

- (2) If $\lambda_n(\vec{z}_0) =: \lambda_0$ is a double eigenvalue, the dispersion relation is given locally by
- (21)
$$\lambda - \lambda_0 = \pm|\alpha||\vec{z} - \vec{z}_0| + o(|\vec{z} - \vec{z}_0|).$$

Note that α may be equal to zero.

Proof. We start by remarking that by standard perturbation theory the number of eigenvalues close to λ_0 in the vicinity of the point \vec{z}_0 remains equal to the multiplicity of λ_0 at \vec{z}_0 .

We know from general theory of analytic Fredholm operators [43] that the dispersion relation is an analytic variety, i.e. given by an equation

$$F(\lambda, \vec{z}) = 0,$$

where F is a real-analytic function. Without loss of generality, consider the point $\vec{z}_0 = 0$. It is an easy special case of Hilbert-Weyl theorem on invariant functions [40] (see also [14, XII.4]), that if a real-analytic function $f(\varkappa_1, \varkappa_2)$ is symmetric with respect to rotations by $2\pi/3$ around the origin, it can be represented as

$$(22) \quad f(\varkappa_1, \varkappa_2) = g(\varkappa_1^2 + \varkappa_2^2, \varkappa_1^3 - 3\varkappa_1\varkappa_2^2, \varkappa_2^3 - 3\varkappa_2\varkappa_1^2)$$

with some real-analytic g .

Therefore, the Taylor expansion for the function F is

$$F(\lambda, \vec{z}) = F_0(\lambda) + F_2(\lambda) |\vec{z}|^2 + o(|\vec{z}|^2).$$

The result now follows from the first terms of expansions of F_0 and F_2 . Indeed, if $F(\lambda, \vec{0})$ has a simple root at $\lambda = \lambda_0$, we have (up to an overall constant)

$$(23) \quad F(\lambda, \vec{z}) = (\lambda - \lambda_0) + a|\vec{z}|^2 + O((\lambda - \lambda_0)^2) + O((\lambda - \lambda_0)|\vec{z}|^2) + O(|\vec{z}|^3).$$

Then, given an ε , $0 < \varepsilon < 1$, there is a small \vec{z} -neighborhood of $\vec{0}$, such that for every \vec{z} the function $F(\lambda, \vec{z})$ changes sign between $\lambda = \lambda_0 + a|\vec{z}|^2 - |\vec{z}|^{2+\varepsilon}$ and $\lambda = \lambda_0 + \alpha|\vec{z}|^2 + |\vec{z}|^{2+\varepsilon}$.

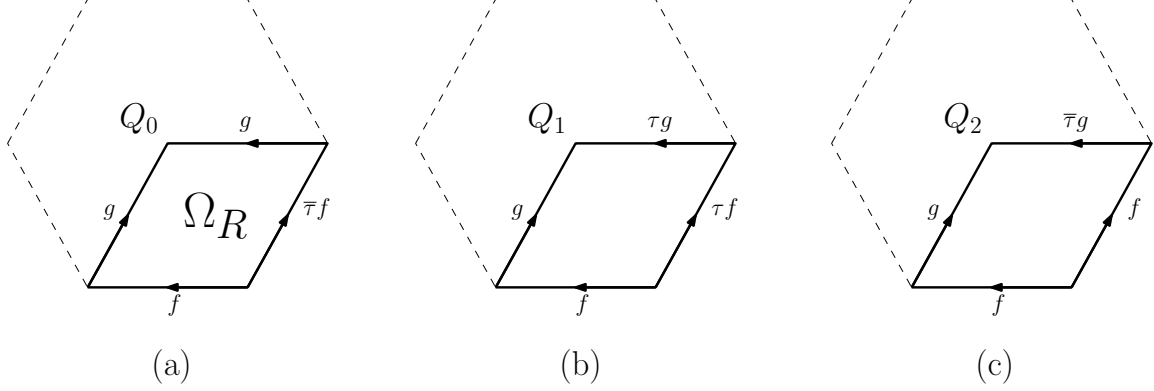


FIGURE 6. Operators Q_0 , Q_1 and Q_2 . We use the notation $\tau = e^{2\pi i/3}$.

Similarly, if $\lambda = \lambda_0$ is a double root, we have

$$(24) \quad F(\lambda, \vec{z}) = (\lambda - \lambda_0)^2 - |\alpha|^2 |\vec{z}|^2 + O((\lambda - \lambda_0)^3) + O((\lambda - \lambda_0) |\vec{z}|^2) + O(|\vec{z}|^3).$$

Note that the coefficient of $|\vec{z}|^2$ cannot be negative since it would make the eigenvalue disappear for non-zero \vec{z} . If $\alpha \neq 0$, the function F changes sign on the interval $\lambda = \lambda_0 + |\alpha| |\vec{z}| \pm |\vec{z}|^{1+\varepsilon}$ and also on the interval $\lambda = \lambda_0 - |\alpha| |\vec{z}| \pm |\vec{z}|^{1+\varepsilon}$. When $\alpha = 0$, a more careful analysis shows that for suitably chosen $\delta > 0$ and $\varepsilon > 0$, the function F is strictly positive in the region $|\vec{z}|^{1+\varepsilon} < |\lambda - \lambda_0| < \delta$ and therefore the dispersion relation must lie in the region $|\lambda - \lambda_0| \leq |\vec{z}|^{1+\varepsilon}$. \square

4. DEGENERACIES IN THE SPECTRUM AT THE POINT $\pm \vec{k}^*$

We will now give a simple proof of the presence of degeneracies in the spectrum of the operator $H(\vec{k})$ at the points $\pm \vec{k}^*$, which forms a part of Theorem 2.1. Our approach is a “transplantation proof”, similar to the proofs of isospectrality of certain domains (such as the proof by Buser et al. [7] for the Gordon–Webb–Wolpert pair [16]). As in isospectrality, while the proof itself is extremely simple, it is a result of a more complicated procedure involving finding irreducible representations of the group of symmetries. The algebra behind the proof (which can be easily extended to other settings) is described in Appendix B.

Consider the rhombic subdomain Ω_R covering 1/3 of the hexagonal fundamental domain, shown in Fig. 6. Denote by Q_j , $j = 0, 1, 2$, the operators having the same differential expression as H (see (2)) and with the boundary conditions specified in Fig. 7(a), (b) and (c), correspondingly.

Theorem 4.1. *Let the self-adjoint operator with real coefficients H be invariant under the shifts by the lattice Γ and the rotation R . The operator $H(\vec{k}^*)$, where $\vec{k}^* := (2\pi/3, -2\pi/3)$, splits into the direct sum*

$$(25) \quad H(\vec{k}^*) \cong Q_0 \oplus Q_1 \oplus Q_2.$$

More precisely, there are three unitary operators $T_j : L^2(\Omega_R) \rightarrow L^2(\Omega_H)$ such that

$$(26) \quad \text{Dom } H(\vec{k}^*) = T_0(\text{Dom } Q_0) \oplus T_1(\text{Dom } Q_1) \oplus T_2(\text{Dom } Q_2),$$

and on $T_j(\text{Dom } Q_j)$, $H(\vec{k}^*)$ restricts to $T_j^* Q_j T_j$, $j = 0, 1, 2$.

If H is also invariant with respect to at least one of the following: reflection F or inversion V , then the operators Q_1 and Q_2 are isospectral.

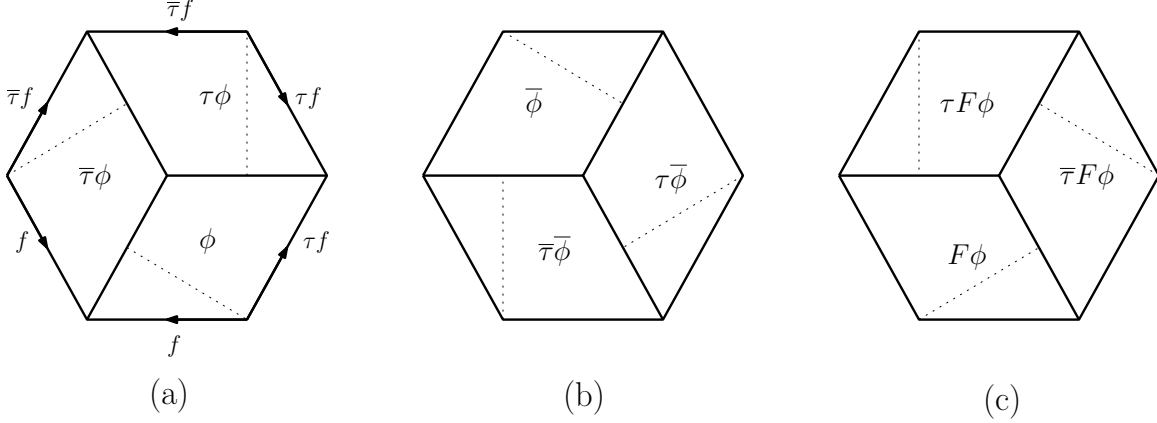


FIGURE 7. Constructing multiple eigenvalues of $H(\vec{k}^*)$. (a) Constructing an eigenfunction of $H(\vec{k}^*)$ out of the eigenfunction of Q_1 . (b,c) Constructing a second eigenfunction using inversion and horizontal reflection symmetries, correspondingly. The dotted lines were added to domains to indicate their orientation.

Proof. To define the unitary operators T_j we embed the functions from $L^2(\Omega_R)$ into $L^2(\Omega_H)$ by extending them by 0 and then let

$$(27) \quad T_0 = \frac{1}{\sqrt{3}} (I + R + R^2), \quad T_1 = \frac{1}{\sqrt{3}} (I + \tau R + \bar{\tau} R^2), \quad T_2 = \frac{1}{\sqrt{3}} (I + \bar{\tau} R + \tau R^2),$$

where R is the operator rotating the function by $2\pi/3$ and

$$(28) \quad \tau := e^{2\pi i/3}.$$

It is now a straightforward check that because of the boundary conditions imposed on the functions from $\text{Dom } Q_j$, they glue smoothly after rotation by R along the internal boundaries and also satisfy the boundary conditions imposed on Ω_H with $\omega_1 = \tau$ and $\omega_2 = \bar{\tau} = \tau^2$, see Fig. 2(b). The operators $\frac{1}{\sqrt{3}}T_j$ can also be considered as acting $L^2(\Omega_H) \rightarrow L^2(\Omega_H)$ in which case they are orthogonal (and mutually orthogonal) projectors, which we will denote P_j .

To prove isospectrality, we start with an eigenfunction ϕ of the operator Q_1 . Applying T_1 we obtain the function depicted in Fig. 7(a), which is an eigenfunction of H . We then apply either \bar{V} or F , depending on which symmetry the operator H has, obtaining Fig. 7(b) or (c) correspondingly. This creates an eigenfunction of H invariant under the action of T_2 . Cutting out the domain Ω_R we obtain an eigenfunction of Q_2 .

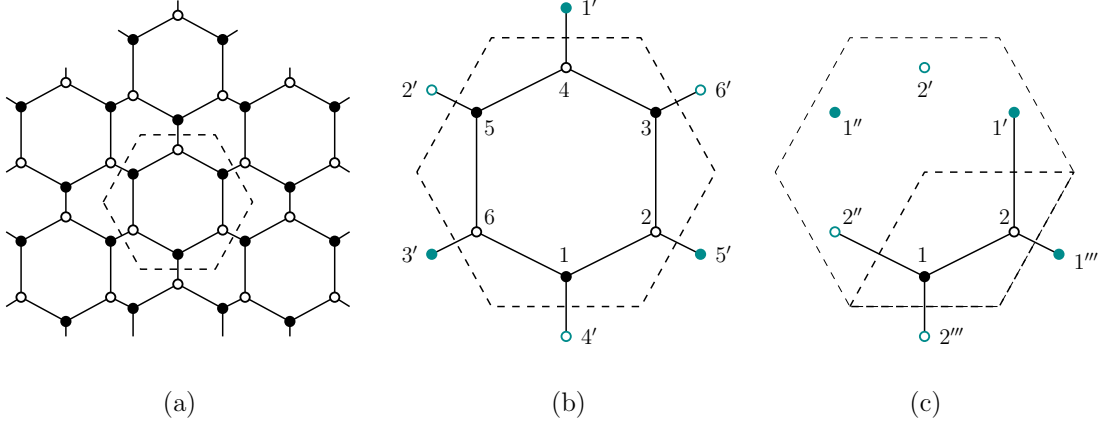
The self-adjointness of Q_j can be obtained, for example, from the self-adjointness of H restricted to the reducing subspace $T_j(\text{Dom } Q_j)$ (see, e.g., [39, Thm 7.28]). The spectra of self-adjoint operators Q_j cannot be empty.

The same result for the point $-\vec{k}^*$ follows from symmetry with respect to complex conjugation, see equation (18) and Corollary 3.2. \square

Remark 4.2. The isospectrality of the operators Q_1 and Q_2 is also checked in Appendix B using an algebraic condition of Band, Parzanchevski and Ben-Shach [4]. The algebraic approach is less elementary but can be more immediately extended to other symmetry groups.

Corollary 4.3. *For any potential, the degenerate eigenstates of $H(\vec{k}^*)$ vanish (are suppressed) at the center of the hexagonal fundamental domain.*

Proof. At the top left corner of the rhombic subdomain, Fig. 6(a), the boundary conditions require $g = \tau g$. This point is fixed by either the reflection or the inversion, thus both eigenfunctions have a zero there. \square

FIGURE 8. A discrete graph with symmetries R and F .

4.1. Graph examples. While the proof of Theorem 4.1 was formulated for continuous differential operators in \mathbb{R}^2 , the method applies to other models, such as graphs, with a little adjustment. Here we explain, by example, the construction of the operators Q_j .

Example 4.4. It is easier to start with an example that has a richer structure, such as the periodic graph of Fig. 8(a). It is assumed that the black and white vertices have different potential, therefore V symmetry is broken, while R and F symmetries are still present.

In part (b) the structure of the graph inside the dashed fundamental domain is magnified. Gray vertices outside of the fundamental domain are obtained by shifts from the corresponding vertices inside. For example, $f_{5'} = \omega_2 f_5$, therefore the operator $H(\vec{k})$ at site 2 acts as

$$(H(\vec{k})f)_2 = (f_2 - f_3) + (f_2 - f_1) + r(f_2 - \omega_2 f_5) + q_2 f_2,$$

where we took the longer sides in the structure of Fig. 8(a) to have weight 1 and the shorter sides weight r (usually, the weight is taken to be inversely proportional to length). The entire operator $H(\vec{k})$ is

$$H(\vec{k}) = \begin{pmatrix} q_1 & -1 & 0 & r\bar{\omega}_1\omega_2 & 0 & -1 \\ -1 & q_2 & -1 & 0 & -r\omega_2 & 0 \\ 0 & -1 & q_1 & -1 & 0 & -r\omega_1 \\ r\omega_1\bar{\omega}_2 & 0 & -1 & q_2 & -1 & 0 \\ 0 & -r\bar{\omega}_2 & 0 & -1 & q_1 & -1 \\ -1 & 0 & r\bar{\omega}_1 & 0 & -1 & q_2 \end{pmatrix},$$

with ω_j defined in (5); above, for simplicity, the potential q was made to absorb the weighted degree of the corresponding vertex.

With $q_1 = \sqrt{3}$, $q_2 = 0$ and $r = \sqrt{7}$, the eigenvalues of $H(\vec{k}^*)$, calculated numerically, are

$$\begin{matrix} -2.5097 & -2.5097 & -1.6753 & 3.4074 & 4.2418 & 4.2418 \end{matrix}$$

To find operator Q acting on the two darker vertices in Fig. 8(c), we retrace the steps of the proof of Theorem 4.1: for the gray vertices we have

$$f_{1'} = \tau f_1, \quad f_{1''} = \bar{\tau} f_1, \quad f_{2''} = \bar{\tau} f_2$$

by rotation and then

$$f_{1'''} = \bar{\tau} f_{1''} = \tau f_1, \quad f_{2'''} = \bar{\tau} f_2$$

by translation (see Fig. 2(c)). We thus get

$$Q = \begin{pmatrix} q_1 & -1 - \bar{\tau} - r\bar{\tau} \\ -1 - \tau - r\tau & q_2 \end{pmatrix}.$$

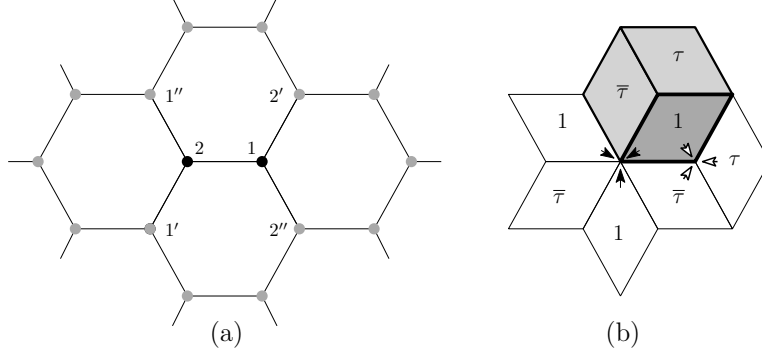


FIGURE 9. Graphene structure with two vertices per fundamental domain.

With the above choice of constants, the eigenvalues of Q are

$$-2.5097 \quad 4.2418$$

which matches the double eigenvalues of $H(\vec{k}^*)$.

Example 4.5. We will now explain the application of our theory to the most basic example: the tight-binding approximation of graphene structure, with vertices of a discrete graph representing carbon atoms, see Fig. 9(a).

The operator $H(\vec{k})$ acts on a 2-dimensional space over vertices 1 and 2 (all other vertices of the graph are obtained by shifts). It acts as

$$\begin{aligned} (H(\vec{k})f)_1 &= -f_2 - f_{2'} - f_{2''} + qf_1 \\ &= -f_2 - \omega_1 f_2 - \omega_2 f_2 + qf_1, \end{aligned}$$

and similarly for $(H(\vec{k})f)_2$. Note that the atoms are identical, hence $q_1 = q_2 = q$. When $\omega_1 = \bar{\omega}_2 = \tau$, the matrix H is q times identity.

The eigenproblem of the rhombic subdomain can be gleaned from Fig. 9(b). In particular, f_1 is forced to be zero: which can be seen from the equality $f_1 = \tau f_1 = \bar{\tau} f_1$ highlighted by the empty arrows in Fig. 9(b), or from the boundary conditions for the bottom right corner of Fig. 7(a). On the other hand, the value f_2 is unrestricted and $(Qf)_2 = qf_2$. The complementary eigenfunction is localized on the vertex 1.

5. CONICAL STRUCTURE AROUND A DEGENERACY

5.1. General perturbation theory. Here we list some general facts from the perturbation theory of operators depending on parameters, following [20, 43, 17]. Let

$$H(r) = H_0 + (r - r_0)H_1 + O(|r - r_0|^2)$$

be an analytic family of self-adjoint operators depending on one parameter with an isolated doubly degenerate eigenvalue λ_0 at $r = r_0$. The eigenvalue then splits into two analytic branches

$$\lambda^\pm(r) = \lambda_0 + \lambda_1^\pm(r - r_0) + O(|r - r_0|^2).$$

The linear terms can be found as the eigenvalues of the 2×2 matrix PH_1P , where P is the projector onto the eigenspace of λ_0 . The corresponding eigenvectors expand as

$$(29) \quad \psi^\pm(r) = \psi_0^\pm + O\left(\frac{|r - r_0|}{|\lambda_1^+ - \lambda_1^-|}\right),$$

where ψ_0^\pm are the eigenvectors of PH_1P (which are in the eigenspace of H_0). All eigenvectors are assumed to be normalized.

If $H = H(k_1, k_2)$ is an analytic function of two parameters and $(0, 0)$ is the point of double multiplicity of the eigenvalue 0, the one-parameter theory is still valid in every direction $k_1 = r \cos(\phi)$, $k_2 = r \sin(\phi)$. The parameters λ_1^\pm now depend on the direction ϕ .

We will say that a doubly degenerate eigenvalue is a conical point if $\lambda_1^+(\phi) \neq \lambda_1^-(\phi)$ in every direction; more precisely,

Definition 5.1. *Let $H(\vec{k})$ be an analytic family of self-adjoint operators. We will say that $H(\vec{k})$ has a nondegenerate conical point at \vec{k}_0 with an eigenvalue λ_0 if $\lambda_0 \in \sigma_d(H(\vec{k}_0))$ is an isolated eigenvalue of geometric multiplicity 2, and in an open neighborhood of \vec{k}_0 the eigenvalues are given by*

$$(30) \quad \lambda^\pm(\vec{k}) = \lambda_0 + (\vec{k} - \vec{k}_0) \cdot \vec{n} \pm \sqrt{Q(\vec{k})} + o(|\vec{k}|),$$

where $\vec{n} \in \mathbb{R}^2$ and $Q(\vec{k})$ is a positive-definite quadratic form. The point \vec{k}_0 is a fully degenerate conical point if the same is true with $Q \equiv 0$.

From Lemma 3.4 we know that the points of double degeneracy at $\pm \vec{k}^*$ and $\vec{0}$ must either be nondegenerate circular cones (in \varkappa coordinates) or fully degenerate cones. It turns out that the point $\vec{0}$ is always a fully degenerate cone; we will also derive a condition for nondegeneracy of the cone at $\pm \vec{k}^*$.

In the first order of perturbation theory, the dispersion surface (i.e. the graph of the eigenvalues as the function of parameters) is given by the solution to⁴

$$(31) \quad \det(k_1 h_1 + k_2 h_2 - \lambda) = 0,$$

where the 2×2 Hermitian matrices h_1 and h_2 are given by

$$(32) \quad h_j = \Phi^* \frac{\partial H}{\partial k_j} \Phi = \begin{bmatrix} \langle f_1, \frac{\partial H}{\partial k_j} f_1 \rangle & \langle f_1, \frac{\partial H}{\partial k_j} f_2 \rangle \\ \langle f_2, \frac{\partial H}{\partial k_j} f_1 \rangle & \langle f_2, \frac{\partial H}{\partial k_j} f_2 \rangle \end{bmatrix}, \quad j = 1, 2.$$

Here $\Phi = [f_1, f_2]$ is a matrix whose columns are the orthonormal basis vectors of the degenerate eigenspace at $(0, 0)$:

$$\Phi : \mathbb{R}^2 \rightarrow \mathcal{X}, \quad \Phi : \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \mapsto c_1 f_1 + c_2 f_2.$$

The projector P onto the eigenspace is then given by $P = \Phi \Phi^*$.

We will now derive matrices h_1 and h_2 explicitly.

5.2. Application to graphene operators. At the singularity points $\pm \vec{k}^*$ we are guaranteed by the construction in the proof of Theorem 4.1 (see Fig. 7(b-d)) to have two orthogonal eigenfunctions f_1 and f_2 such that

$$(33) \quad R f_1 = \tau f_1, \quad R f_2 = \bar{\tau} f_2.$$

The existence of such eigenfunctions also follows directly from representation theory, equations (63) and (73) in the Appendix. Using this basis for the eigenspace results in a simple form for the derivatives h_j , $j = 1, 2$.

Theorem 5.2. *In the basis $\{f_1, f_2\}$ satisfying (33), the matrices h_1 and h_2 are given by*

$$(34) \quad h_1 = \begin{pmatrix} 0 & \alpha \\ \bar{\alpha} & 0 \end{pmatrix}, \quad h_2 = \begin{pmatrix} 0 & \tau \alpha \\ \bar{\tau} \alpha & 0 \end{pmatrix},$$

⁴This is a standard procedure in quantum mechanics or solid state physics (known as $k \cdot p$ method in the latter); for a mathematical proof, see [17].

where, by the definition (32),

$$(35) \quad \alpha = \left\langle f_1, \frac{\partial H}{\partial k_1} f_2 \right\rangle.$$

Remark 5.3. This calculation was performed for \mathbb{R}^2 Laplacian with any R -symmetric potential in [12, Prop 4.2], using explicit calculation of the derivatives $\partial H / \partial k_j$. We give a general derivation in the spirit of the Hilbert-Weyl theory of invariant functions.

Proof. From Lemma 3.1 we have

$$R \left(H(\vec{k}^* + \vec{k}) - H(\vec{k}^*) \right) R^* = H \left(\hat{R}(\vec{k}^* + \vec{k}) \right) - H \left(\hat{R}\vec{k}^* \right) = H \left(\vec{k}^* + \hat{R}\vec{k} \right) - H \left(\vec{k}^* \right),$$

where we used the fact that \vec{k}^* is a fixed point of (14). Passing to the limit, we get

$$(36) \quad R \left(D_{\vec{k}} H \right) R^* = D_{\hat{R}\vec{k}} H,$$

where by $D_{\vec{k}} H := k_1 \partial_{k_1} |_{\vec{k}^*} H + k_2 \partial_{k_2} |_{\vec{k}^*} H$ we denote the directional derivative of H at the point \vec{k}^* .

Introduce the notation

$$h_{\vec{k}} := \Phi^* \left(D_{\vec{k}} H \right) \Phi = k_1 h_1 + k_2 h_2.$$

Conjugating equation (36) by the matrix Φ , we get

$$(37) \quad \rho(R)^T h_{\vec{k}} \rho(R^*)^T = h_{\hat{R}\vec{k}},$$

where $\rho(R^*)$ is the matrix representation of the rotation $R^* = R^{-1}$ defined by its action in the eigenspace $\text{span}(f_1, f_2)$, namely

$$R^*[f_1, f_2] = [f_1, f_2] \rho(R^*)^T$$

(compare with equation (58) and other material in Appendix B).

In our choice of basis (see equation (33)), one has $R^*(f_1, f_2) = (\bar{\tau} f_1, \tau f_2)$, therefore

$$\rho(R^*)^T = \begin{pmatrix} \bar{\tau} & 0 \\ 0 & \tau \end{pmatrix}.$$

Using the explicit form of the matrix \hat{R} from (12), equation (37) can be written in components as

$$(38) \quad \begin{pmatrix} \tau & 0 \\ 0 & \bar{\tau} \end{pmatrix} h_1 \begin{pmatrix} \bar{\tau} & 0 \\ 0 & \tau \end{pmatrix} = -h_1 - h_2, \quad \begin{pmatrix} \tau & 0 \\ 0 & \bar{\tau} \end{pmatrix} h_2 \begin{pmatrix} \bar{\tau} & 0 \\ 0 & \tau \end{pmatrix} = h_1.$$

It is now straightforward to check that any 2×2 Hermitian matrices satisfying (38) must be of the form (34). \square

From expressions (34) one can explicitly calculate the shape of the dispersion relation in the first order of perturbation theory using (31). It is

$$(39) \quad \lambda^2 - |\alpha|^2 |k_1 + \tau k_2|^2 = \lambda^2 - \frac{4}{3} |\alpha|^2 |\mathcal{Z}|^2 = 0,$$

where we changed to the coordinates

$$(40) \quad \vec{\mathcal{Z}} = k_1 \vec{b}_1 + k_2 \vec{b}_2,$$

in which the dispersion relation is the circular cone with no tilt. It becomes degenerate if $\alpha = 0$ (this condition is equivalent to condition (4.1) of [12]). In [17], α was shown to be non-zero for small potential, therefore, if the potential strength is controlled by a parameter, the cone can be degenerate only for isolated values of the parameter. We explore this in more detail in the next section.

5.3. Perturbation of the pure Laplacian. In this section we describe in more detail the case of Laplacian on \mathbb{R}^2 with the potential considered as a perturbation, $H_\varepsilon = -\Delta + \varepsilon q(\vec{x})$. Similar calculation appeared in [17] and [12] (see also [11]), therefore we concentrate on connections with the results presented above.

Proof of Theorem 2.2. When $\varepsilon = 0$, the lowest eigenvalue of $H_0(\vec{k}^*)$ is triply degenerate. Indeed, the function

$$(41) \quad \phi(\vec{x}) := \exp(i\vec{\mathcal{K}}^* \cdot \vec{x}) = \exp\left(\frac{4\pi i}{3}x_2\right)$$

is an eigenfunction of the Laplacian and satisfies

$$\phi(\vec{x} + \vec{a}_1) = \tau\phi(\vec{x}), \quad \phi(\vec{x} + \vec{a}_2) = \bar{\tau}\phi(\vec{x}),$$

therefore it is an eigenfunction of $H_0(\vec{k}^*)$. Since R , the operator of rotation by $2\pi/3$, commutes with $H_0(\vec{k}^*)$, the functions

$$(42) \quad R\phi = \exp\left(\frac{4\pi i}{3}\left(-\frac{\sqrt{3}}{2}x_1 - \frac{1}{2}x_2\right)\right), \quad R^2\phi = \exp\left(\frac{4\pi i}{3}\left(\frac{\sqrt{3}}{2}x_1 - \frac{1}{2}x_2\right)\right),$$

are also eigenfunctions. It can be verified directly that they are orthogonal. Their combinations

$$(43) \quad \psi_j(\vec{x}) := \frac{1}{3}(\phi(\vec{x}) + \tau^j R\phi(\vec{x}) + \bar{\tau}^j R^2\phi(\vec{x})) = P_j\phi, \quad j = 0, 1, 2,$$

are simple eigenfunctions of the operators Q_j from Fig. 6 for $j = 0, 1, 2$ correspondingly (see also the discussion following equation (27)).

We now need to show that the eigenvalues of Q_0 and Q_1 (or Q_2) will separate for non-zero ε . In the first order perturbation theory, the condition for separation is

$$(44) \quad \frac{\langle \psi_0, q(\vec{x})\psi_0 \rangle}{\langle \psi_0, \psi_0 \rangle} \neq \frac{\langle \psi_1, q(\vec{x})\psi_1 \rangle}{\langle \psi_1, \psi_1 \rangle} = \frac{\langle \psi_2, q(\vec{x})\psi_2 \rangle}{\langle \psi_2, \psi_2 \rangle}$$

where the scalar products are taken in $L^2(\Omega_R)$. Since the functions $\overline{\psi_j(\vec{x})}q(\vec{x})\psi_j(\vec{x})$ are R -invariant and $\|\psi_0\| = \|\psi_1\| = \|\psi_2\|$, condition (44) is equivalent to

$$(45) \quad \langle P_0\phi, q(\vec{x})P_0\phi \rangle_{L^2(\Omega_H)} + \tau \langle P_1\phi, q(\vec{x})P_1\phi \rangle_{L^2(\Omega_H)} + \bar{\tau} \langle P_2\phi, q(\vec{x})P_2\phi \rangle_{L^2(\Omega_H)} \neq 0.$$

Using that P_j are projectors which commute with multiplication by the R -invariant function $q(x)$, we reduce the left-hand side to

$$(46) \quad \langle (P_0 + \bar{\tau}P_1 + \tau P_2)\phi, q(\vec{x})\phi \rangle = \langle R\phi, q\phi \rangle = \langle R^2\phi, qR\phi \rangle = \int_{\Omega_H} e^{\frac{4\pi i}{\sqrt{3}}x_1} q(\vec{x}) d\vec{x}.$$

Two more facts are now needed to establish existence of non-degenerate conical points for almost all values of $\varepsilon > 0$.

- (1) The parameter α describing the opening angle of the cone, see equations (35) and (39), is analytic as a function of ε .
- (2) α is nonzero when $\varepsilon = 0$.

Analyticity of $\alpha = \alpha(\varepsilon)$ follows from the analyticity of the eigenfunction corresponding to a simple eigenvalue of the self-adjoint operator $Q_1(\varepsilon)$ as a function of one parameter; this is a consequence of the results of Rellich and Kato, see [20, Sec. VII.3] and [32]. The eigenfunctions f_1 and f_2 in the definition of α (cf. (35)), are obtained from the eigenfunction of Q_1 by the unfolding prescribed by Fig. 7, and are therefore also analytic, while the derivative $\partial H / \partial k_1 = \partial H_0 / \partial k_1$ does not depend on ε .

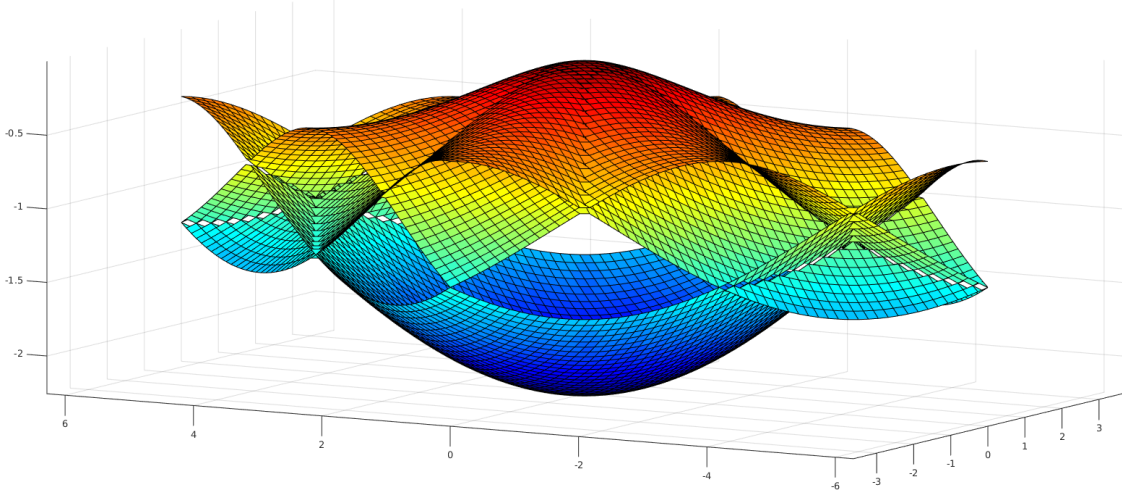


FIGURE 10. The lower three sheets of the dispersion relation for the graph in Example 4.4 with the parameter $r = 1$.

Finally, we calculate the value of $\alpha(0) \neq 0$ explicitly. By the standard gauge transformation technique, $D_{\vec{k}}H = -2i\vec{k} \cdot \nabla$. Therefore,

$$(47) \quad \alpha = \frac{1}{\|\psi_1\|\|\psi_2\|} \left\langle \psi_1, \frac{\partial H}{\partial k_1} \psi_2 \right\rangle_{L^2(\Omega_H)} = \frac{-2i}{\|\psi_1\|\|\psi_2\|} \left\langle \psi_1, \frac{\partial}{\partial x_1} \psi_2 \right\rangle$$

$$(48) \quad = \frac{-2i}{\|\phi\|^2} \left\langle \phi + R\phi + R^2\phi, \frac{\partial}{\partial x_1} (\phi + \tau R\phi + \tau^2 R^2\phi) \right\rangle$$

$$(49) \quad = \frac{-2i}{\|\phi\|^2} \left\langle \phi + R\phi + R^2\phi, -\frac{2\pi i}{\sqrt{3}}\tau R\phi + \frac{2\pi i}{\sqrt{3}}\tau^2 R^2\phi \right\rangle = \frac{4\pi}{\sqrt{3}}(-\tau + \tau^2) = -4\pi i.$$

using formulas for ψ_1 and ψ_2 and orthogonality of ϕ , $R\phi$ and $R^2\phi$. \square

Remark 5.4. Consider a potential $q(\vec{x})$ which is R -invariant, but may not have V or F symmetry. It can be shown that the first order perturbation condition for the eigenvalues of Q_1 and Q_2 to *not separate* is precisely that the right hand side of equation (46) is real. The latter is of course satisfied if $q(\vec{x})$ does have V or F symmetry.

Example 5.5. To continue with Example 4.4, it is interesting to investigate⁵ what happens when the parameter r is equal to 1. At the special points $\pm\vec{k}^*$ there are now triple degeneracies as the spectrum of Q_0 coincides at this point with the spectra of Q_1 and Q_2 . As a consequence there is no conical point there. Instead, the lower 3 sheets of the dispersion relation develop singularities along curves and touch each other to form an intricate picture, Figure 10. The picture can be resolved as three analytic surfaces crossing each other. Similar shape is assumed by the upper 3 sheets.

The reason for such a complicated picture is that the system now has more symmetry and the three sheets can be obtained by (1) considering the smaller fundamental domain, (2) cutting up its dispersion relation and folding it back to Brillouin zone chosen in Figure 10. This is analogous to the situation with H_0 above which has more symmetry than the hexagonal lattice. It also illustrates the observation of [12] that the cones may degenerate at isolated values of a parameter (r , in the present example).

⁵This question was asked by P. Kuchment.

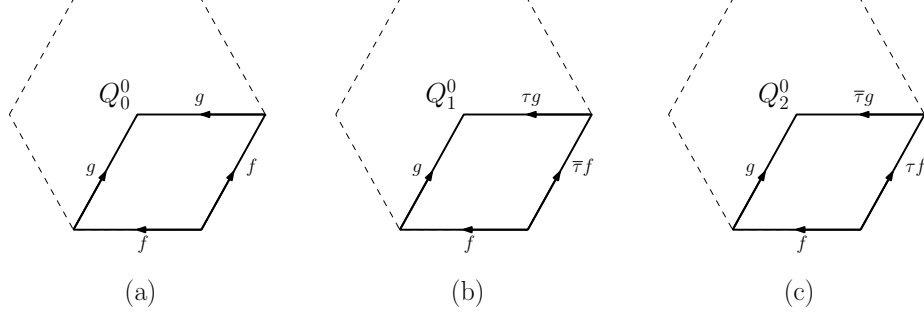


FIGURE 11. The operators Q_j^0 that together give the spectrum of $H(\vec{0})$.

6. DEGENERACY AT $\vec{k} = \vec{0}$

The third fixed point of the rotation \hat{R} in the momentum space (see (15) in Lemma 3.1) also leads to degeneracies in the spectrum. They are present even if both inversion and reflection symmetries are broken: rotation and complex conjugation are sufficient to retain degeneracies. However, the local structure of the dispersion relation is not conical, see Fig. 4 for an example.

Theorem 6.1. *Let the self-adjoint operator with real coefficients H be invariant under the shifts by the lattice Γ and the rotation R . Then the operator $H(\vec{0})$ splits into the direct sum*

$$(50) \quad H(\vec{k}^*) \cong Q_0^0 \oplus Q_1^0 \oplus Q_2^0,$$

where the operators Q_1^0 and Q_2^0 are isospectral.

If $\lambda = \lambda_0$ is a simple eigenvalue of Q_1^0 and is not an eigenvalue of Q_0^0 , then the dispersion relation is locally flat at $\vec{k} = \vec{0}$:

$$(51) \quad (\lambda - \lambda_0)^2 = o(|\vec{k}|^2).$$

Remark 6.2. The eigenvalue $\lambda_1(\vec{0})$ is always non-degenerate, therefore first and second bands cannot touch at $\vec{k} = \vec{0}$.

Proof. The proof of the first part is identical to the proof of Theorem 4.1 with operators Q_j^0 , $j = 0, 1, 2$, shown in Fig. 11. To show isospectrality, we start with an eigenfunction ϕ of Q_1^0 , unfold it using the operator T_1 , equation (27), apply the complex conjugation and restrict it back to the domain Ω_R , obtaining an eigenfunction of Q_2^0 . In this way we obtain two eigenfunctions of $H(\vec{0})$: $f_1 = T_1\phi$ and $f_2 = \overline{f_1}$.

For the second part, the proof of Theorem 5.2 still applies so the matrices h_1 and h_2 have the form given by (34). Repeating the proof for the complex conjugation (or “time reversal”) C as a symmetry of $H(\vec{k})$ at $\vec{k} = \vec{0}$ (in place of R), we arrive at the following analogue of (37):

$$(52) \quad \overline{\rho(C)^T h_{\vec{k}} \rho(C^{-1})^C} = h_{-\vec{k}}.$$

The overall complex conjugation arises because C is antiunitary. Since complex conjugation maps f_1 and f_2 to each other,

$$\rho(C) = \rho(C^{-1}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

From (52) and the fact that $h_{\vec{k}}$ is Hermitian, we obtain that $h_{\vec{k}}$ is necessarily diagonal (and also has trace 0). Comparing with (34), we conclude that $h_{\vec{k}} \equiv 0$. \square

Remark 6.3. More generally, one can get the following result. Suppose the operator $H(\vec{k}) = H(k_1, k_2)$ has the following symmetry at the point \vec{k}_0 :

$$H(\vec{k}_0 - \vec{k}) = \overline{H(\vec{k}_0 + \vec{k})} := CH(\vec{k}_0 + \vec{k})C^{-1}.$$

If λ_0 is an eigenvalue of $H(\vec{k}_0)$ of multiplicity 2, it cannot be a nondegenerate conical point. In the leading order, it must have the form of two intersecting planes of which (51) is a degenerate example.

Example 6.4. Revisiting Example 4.4 and calculating the eigenvalues of $H(\vec{0})$ numerically, we get

$$-3.8598 \quad -0.9937 \quad -0.9937 \quad 2.7257 \quad 2.7257 \quad 5.5918$$

The corresponding operator Q_0 in this case can be shown to be

$$Q_0 = \begin{pmatrix} q_1 & -1 - \bar{\tau} - r\tau \\ -1 - \tau - r\bar{\tau} & q_2 \end{pmatrix}.$$

with eigenvalues -0.9937 and 2.7257 .

Interestingly, in the case of Example 4.5, the graph structure is not rich enough to support the operator Q_0 : it can be shown that the only lattice-periodic function that can be represented as $T_0\phi$ must have $f_1 = f_2 = 0$.

In Appendix C we give a brief account of the case of pure Laplacian on \mathbb{R}^2 at the quasimomentum point $\vec{k} = 0$. It is largely parallel to Section 5.3, but requires more tools from representation theory, introduced in Appendix B.

7. PERSISTENCE OF CONICAL POINTS

We are now going to consider whether the conical point survives when the rotational symmetry is broken by a small perturbation. We will consider two cases when the perturbation retains the inversion V or the reflection F symmetry (all other symmetries may or may not be broken). In both cases the conical point survives. Moreover, in the second case we are able to restrict the location of the surviving point to a line in \vec{k} space. Of course, if the perturbation retains both symmetries, V and F , the stronger second result still applies.

7.1. Keeping V symmetry: Berry phase. Let us consider the weakly broken R symmetry: we add to H a perturbation which is V -invariant but not R -invariant. The F symmetry may or may not be preserved.

The tool for proving Theorem 2.3 in this case is the “Berry phase” [5, 33] (also known as “Pancharatnam–Berry phase” or “geometric phase”), of which we first give an informal description. Consider choosing a closed contour in the parameter space and tracking certain eigenvalue along this contour. The eigenvalue changes as we move along the contour, but we assume it remains simple. Now we choose the corresponding normalized eigenvector at every point of the contour. The eigenvector is defined up to a phase, and we choose it “in the most continuous fashion”. Once we completed the loop, the final eigenvector must equal the initial eigenvector up to a phase factor $e^{i\phi}$. The phase ϕ we call the Berry phase. The fact that it might be different from zero (modulo 2π) in the simplest form of real operator H and a contour encircling a conical point has been known for a while, see [19] and [1, Appendix 10.B].

We now argue that the Berry phase of the operator $H_\varepsilon(\vec{k})$ is restricted to only take values 0 or π (modulo 2π). Because of the symmetry of the perturbation W , the perturbed operator $H_\varepsilon(\vec{k})$ will retain the symmetry \bar{V} for all \vec{k} . The operator \bar{V} is an antiunitary involution, i.e.

$$(53) \quad \bar{V}(\alpha v) = \bar{\alpha}(\bar{V}v), \quad \bar{V}^2 = 1, \quad \langle \bar{V}v, \bar{V}u \rangle = \langle u, v \rangle.$$

If ψ is a simple eigenfunction of $H(\vec{k})$, then, after multiplication by a suitable phase,

$$(54) \quad \bar{V}\psi := \overline{\psi(-\vec{x})} = \psi.$$

Indeed, because \bar{V} commutes with the operator $H(\vec{k})$, $\overline{\psi(-\vec{x})}$ is an eigenvector with the same eigenvalue and thus equal to $e^{i\theta}\psi$ for some θ . Multiplying ψ by $e^{i\theta/2}$ makes it satisfy equation (54).

Condition (54) gives us a canonical way to choose the overall phase of the eigenvector, up to a sign.⁶ Now consider a closed path in the parameter \vec{k} space. The phase acquired by a parallel section of the eigenspaces (the formal definition of the Berry phase) is restricted by condition (54): the factor must be either $+1$ or -1 , so the phase is either 0 or π modulo 2π .

On the other hand, the phase must change continuously upon a continuous deformation of the contour. Therefore, if the contour is homotopically equivalent to a point (i.e. encloses no parameter values where the eigenvalue becomes multiple), the phase must be equal to zero. But if the contour encloses a conical point, the phase is equal to $\pi \pmod{2\pi}$.

Lemma 7.1. *Let the self-adjoint operator $H(\vec{k})$, which analytically depends on the two parameters $\vec{k} = (k_1, k_2)$, have a nondegenerate conical point at $(0, 0)$. Let $H(\vec{k})$ commute with an antiunitary involution \bar{V} . Then the Berry phase acquired on a contour enclosing the singularity $(0, 0)$ is π .*

Remark 7.2. This result for a real-valued operator H can be traced back at least to Herzberg and Longuet-Higgins [19]. Their proof is based on reducing the question using perturbation theory to a question about 2×2 matrices and computing the eigenvectors explicitly. A more general formula is derived in [5, Sec. 3], from which Lemma 7.1 follows. In Appendix E we include an alternative derivation which avoids computing anything explicitly, opting instead for a more geometric explanation, which has interesting similarities to considerations of Section 7.2.

From this we immediately conclude that an isolated non-degenerate conical point cannot disappear under a perturbation which preserves the above symmetry.

Proof of Theorem 2.3 when \bar{V} symmetry. Surround the point with a small contour γ , such that inside this contour the eigenvalue $\lambda_-(\vec{k})$ of $H_{\varepsilon=0}(\vec{k})$, see (30), is simple except at \vec{k}^* . Then on contour γ the Berry phase of the corresponding eigenfunction must be π .

For small values of ε , the eigenvalue on the contour γ remains simple (as a continuous function on a compact set). Therefore, the phase must change continuously, so it must remain constant. Finally, if there were no multiplicity of $\lambda_{-, \varepsilon}(\vec{k})$ inside the contour, the Berry phase would be 0 . The multiplicity gives rise to a nondegenerate conical point by continuity. \square

7.2. Keeping F symmetry: parity exchange. Let us now consider the weakly broken R symmetry: we add to H a perturbation which is F -invariant but not R -invariant. The V symmetry may or may not be preserved.

Proof of Theorem 2.3 with F symmetry. As explained in Section 3, F remains a symmetry of the operator $H(\vec{k})$ when the quasimomenta \vec{k} satisfy $\omega_2 = \bar{\omega}_1$ or, equivalently, $k_2 = -k_1$ modulo 2π .

Since the subgroup generated by F has two representations, the space $\mathcal{X}(\vec{k})$ decomposes into two orthogonal subspaces, even and odd, defined by

$$(55) \quad \mathcal{X}_F^+ = \{\psi \in \mathcal{X}(\vec{k}) : F\psi = \psi\} \quad \text{“even”},$$

$$(56) \quad \mathcal{X}_F^- = \{\psi \in \mathcal{X}(\vec{k}) : F\psi = -\psi\} \quad \text{“odd”}.$$

All simple eigenvectors of $H_\varepsilon(\vec{k})$ on the symmetry line belong to one or the other subspace. Multiple eigenspaces admit a basis consisting of vectors, each of which is either odd or even.

⁶This choice of the eigenvector along a curve in the parameter space defines a parallel section of the line bundle of the eigenspaces.

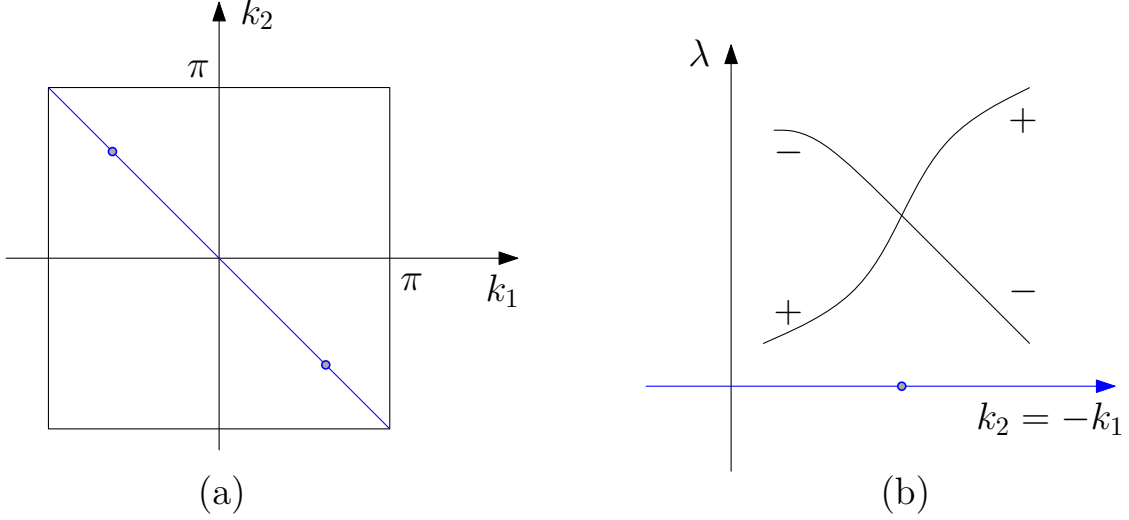


FIGURE 12. The line in the Brillouin zone where the symmetry F is preserved (a). The form of the dispersion relation along the symmetry line (b).

Now suppose we are at the special symmetry point \vec{k}^* in the presence of rotational symmetry R (i.e. $\varepsilon = 0$). At the conical point we have a doubly degenerate eigenvalue with orthogonal eigenvectors described by Fig. 7(a) and (c). It can be seen directly that the sum of these eigenvectors is even and the difference is odd with respect to F .

Now consider the restrictions of the operator H_ε with $\varepsilon = 0$ onto the two subspaces \mathcal{X}_F^+ and \mathcal{X}_F^- . The above consideration shows that at the special point each restriction has a simple eigenvalue. As we go along the line $k_2 = -k_1$, the eigenvalue of each restriction is an analytic function. These functions have an intersection at the point $k_1 = -k_2 = 2\pi/3$. Since the two functions form a section of a non-degenerate cone, the intersection is transversal, see Fig. 12(b). Such intersection is stable under perturbation, and therefore, when we consider small $\varepsilon \neq 0$ (keeping the symmetry F), the intersection survives. Moreover, we know it remains on the line $k_2 = -k_1$ and the only way it can disappear is by colliding with another degenerate eigenvalue on this line.

The intersection corresponds to a degenerate eigenvalue of the operator $H_\varepsilon(k)$ which, for small perturbations of the original potential, must still be a non-degenerate conical point. \square

7.3. Destroying all symmetry. When a perturbation breaks all of the symmetries R , V and F , the conical point normally separates into two surfaces, locally a two-sheet hyperboloid. This was discussed in detail in [12, Remark 9.2]. We merely remark here that the tips of the sheets of the hyperboloid give rise to the edges of the band spectrum. This provides an example for the band edges coming from a point in the bulk of the Brillouin zone, with no additional symmetries (since they have been broken), a subject first addressed on the mathematical level in [18, 10].

APPENDIX A. MATRICES OF SYMMETRY TRANSFORMATIONS

In this section we discuss different coordinates for the position and dual spaces and calculate the matrix \hat{R} (see the definition (12)) in those coordinates. The considerations are very basic, but can be useful for avoiding confusion.

There are two sets of coordinates of the position space: the rectangular Cartesian $\vec{x} = (x_1, x_2)^T$ and coordinates with respect to the basis of the lattice-defining vectors \vec{a}_1, \vec{a}_2 . The latter coordinates we will denote $\vec{\xi} = (\xi_1, \xi_2)^T$. The connection between the two sets is

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \xi_1 \vec{a}_1 + \xi_2 \vec{a}_2 = \begin{pmatrix} \sqrt{3}/2 & \sqrt{3}/2 \\ 1/2 & -1/2 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} =: A\vec{\xi}.$$

The inverse matrix A^{-1} is

$$A^{-1} = \begin{pmatrix} 1/\sqrt{3} & 1 \\ 1/\sqrt{3} & -1 \end{pmatrix} = \begin{pmatrix} \vec{b}_1 \\ \vec{b}_2 \end{pmatrix}.$$

The $\vec{\xi} = (\xi_1, \xi_2)$ coordinates are more convenient for the description of the hexagonal lattice, while $\vec{x} = (x_1, x_2)$ coordinates are slightly more convenient for the description of symmetries: for example the rotation is given by a unitary matrix. Namely, $R\psi(\vec{x}) = \psi(M_R\vec{x})$, where

$$M_R = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

is the matrix of rotation by $2\pi/3$ in the *clockwise* (negative) direction. As usual, to rotate the *function* in the positive direction, we rotate the variables it depends upon in the negative direction.

In terms of coordinates $\vec{\xi}$ we therefore have $R\psi(\vec{\xi}) = \psi(A^{-1}M_RA\vec{\xi})$, where

$$A^{-1}M_RA = \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix},$$

which is, of course, still a rotation by $-2\pi/3$ in terms of the basis (\vec{a}_1, \vec{a}_2) .

The coordinates \vec{k} are dual to $\vec{\xi}$ and therefore the action of R on \vec{k} is given by

$$\hat{R} = (A^{-1}M_RA)^*,$$

which agrees with equation (12).

Finally, one can also use Cartesian coordinates in the dual space. As mentioned before, those are

$$\vec{\varkappa} = k_1\vec{b}_1 + k_2\vec{b}_2 = \begin{pmatrix} 1/\sqrt{3} & 1/\sqrt{3} \\ 1 & -1 \end{pmatrix} \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = B \begin{pmatrix} k_1 \\ k_2 \end{pmatrix},$$

where

$$B = (\vec{b}_1, \vec{b}_2) = (A^{-1})^*.$$

Therefore, in coordinates $\vec{\varkappa}$ the action of R is given by

$$B\hat{R}B^{-1} = M_R^*,$$

a unitary matrix.

For the dual of the horizontal reflection we have

$$\hat{F}_k = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

in k coordinates and

$$\hat{F}_{\varkappa} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = B\hat{F}_kB^{-1}$$

in \varkappa coordinates. As before, $\hat{F}_{\varkappa} = (M_F)^*$, where M_F defines the horizontal reflection in the x coordinates: $F\psi(\vec{x}) = \psi(M_F\vec{x})$.

APPENDIX B. REPRESENTATIONS, DEGENERACIES IN THE SPECTRUM AND ISOSPECTRALITY

B.1. Subspace carrying a representation. Let H be a self-adjoint operator (“Hamiltonian”) acting on a separable Hilbert space \mathcal{X} . Let $\mathcal{S} = \{\text{Id}, S_1, \dots\}$ be a finite group of unitary operators on \mathcal{X} which commute with H (are “symmetries” of H).

Remark B.1. It is assumed implicitly that the domain of H is invariant under the action of operators $S \in \mathcal{S}$. Such technical details will be omitted unless they have some importance to the task at hand.

It is well-known (see, e.g. [15]) that in the circumstances described above, there is an *isotypic decomposition* of \mathcal{X} into a finite orthogonal sum of subspaces each carrying copies of a representation of \mathcal{S} . More precisely,

$$\mathcal{X} = \bigoplus_{\rho} \mathcal{X}_{\rho},$$

where for any two vectors $v_1, v_2 \in \mathcal{X}_{\rho}$, there is an isomorphism between the spaces

$$[\mathcal{S}v_1] = \text{span} \{Sv_1 : S \in \mathcal{S}\} \quad \text{and} \quad [\mathcal{S}v_2] = \text{span} \{Sv_2 : S \in \mathcal{S}\},$$

which preserves the group action on the spaces (i.e. commutes with all $S \in \mathcal{S}$).

For each $v \in \mathcal{X}_{\rho}$, the finite-dimensional subspace $[\mathcal{S}v]$ is an irreducible representation of \mathcal{S} : if it were reducible (i.e. had a proper subspace invariant with respect to \mathcal{S}), there would be $u \in [\mathcal{S}v] \subset \mathcal{X}_{\rho}$, such that $[\mathcal{S}u]$ is a proper subspace of $[\mathcal{S}v]$ and therefore not isomorphic to it. The components \mathcal{X}_{ρ} are maximal: different components correspond to different representations. Thus ρ can be understood as labeling irreducible representations. The dimension of $[\mathcal{S}v]$ is called the dimension of the representation ρ .

Example B.2. Let $\mathcal{X} = L^2(\mathbb{R})$ and \mathcal{S} be the cyclic group of order 2 generated by the reflection $x \mapsto -x$ or, more precisely,

$$S : f(x) \mapsto f(-x).$$

Then $\mathcal{X} = \mathcal{X}_{\text{even}} \oplus \mathcal{X}_{\text{odd}}$, where

$$\mathcal{X}_{\text{even}} = \{f \in \mathcal{X} : f(-x) = f(x)\}, \quad \mathcal{X}_{\text{odd}} = \{f \in \mathcal{X} : f(-x) = -f(x)\}.$$

Then $\mathcal{X}_{\text{even}}$ carries infinitely many copies of the *trivial* representation of \mathcal{S} :

$$\text{Id} \mapsto (1), \quad S \mapsto (1),$$

while \mathcal{X}_{odd} carries infinitely many copies of the *alternating* representation of \mathcal{S} :

$$\text{Id} \mapsto (1), \quad S \mapsto (-1).$$

Both representations are one-dimensional. Note that the decomposition of a \mathcal{X}_{ρ} into irreducible copies is not unique.

Each isotypic component \mathcal{X}_{ρ} is invariant with respect to H : either $Hv = 0$ or H provides the isomorphism between subspaces $[\mathcal{S}v]$ and $[\mathcal{S}Hv]$.

If H has discrete spectrum then the restriction of H to \mathcal{X}_{ρ} has eigenvalues with multiplicities divisible by the dimension of ρ . Indeed, by commuting \mathcal{S} and H we see that if v is an eigenvector of H , then the entire subspace $[\mathcal{S}v]$ is an eigenspace of H with the same eigenvalue.

It is sometimes stated in the physics literature that if the group of symmetries of an operator has an irreducible representation ρ , the operator will have eigenspaces carrying this irreducible representation; in particular, the corresponding eigenvalue will have multiplicity equal to the dimension of ρ . This is not completely correct, as the isotypic component corresponding to this representation can be absent from the domain of operator, due to natural (see [4, Sec. 7.2] for an example) or artificial reasons (e.g. the operator may be restricted to another isotypic component). Thus the fundamental question in describing spectral degeneracies is finding the isotypic decomposition of the domain of the operator.

Instead of performing this task head-on for each set of symmetries, we first do isotypic decomposition with respect to the subgroup of rotations, common to all sets, and then study induced representations.

We also give an advance warning that some of our symmetries act on the Hilbert space \mathcal{X} as antiunitary operators, i.e. operators A satisfying

$$(57) \quad A(\alpha v) = \bar{\alpha}(Av), \quad \langle Av, Au \rangle = \langle u, v \rangle.$$

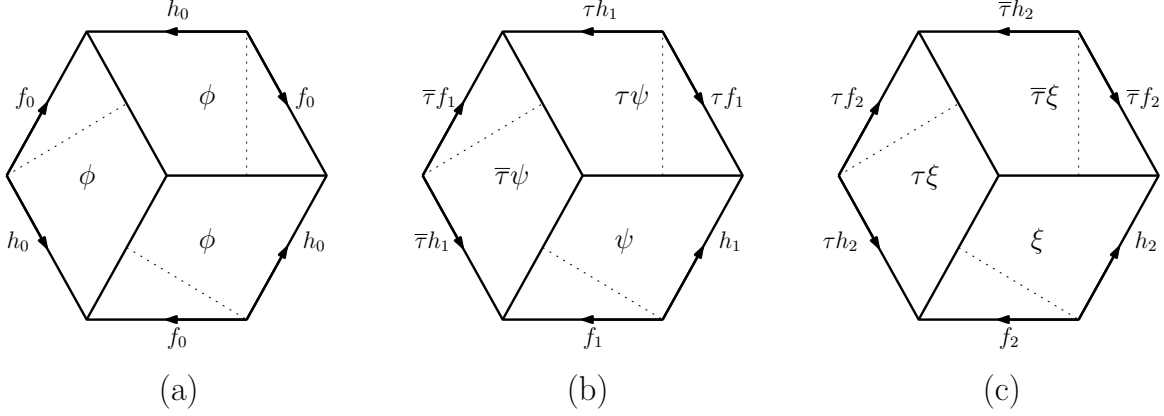


FIGURE 13. Isotypic decomposition of $\mathcal{X}(\vec{k}^*)$ with respect to the representations of the group of rotations by $2\pi/3$.

In such a case the representations need also be in terms of antiunitary matrices; these are the so-called “corepresentations” of Wigner [41] (also known as the “unitary-antiunitary” representations, see, for example, [29]).

B.2. Quotient by the rotation subgroup. Restricting an operator to an isotypic component is the essence of the technique of “taking the quotient of an operator by a representation”, applied in [4, 30] to constructing isospectral graphs and domains (the method is itself a generalization of the so-called Sunada method [35]). We recast their method below as a description of *equivariant vectors* (cf. [44, Def 1.19]).

An isotypic component is spanned by the vectors that transform according to a given representation. To put it formally, for a n -dimensional representation ρ , we are looking to characterize n -tuples of vectors from our Hilbert space \mathcal{X} such that

$$(58) \quad (S\phi_1, \dots, S\phi_n) = (\phi_1, \dots, \phi_n)\rho(S)^T,$$

for each $S \in \mathcal{S}$. The right-hand side should be interpreted as matrix multiplication of a $\dim(\mathcal{X}) \times n$ matrix by an $n \times n$ matrix.

We will take the quotient of the operator $H(\vec{k}^*)$, with respect to representations of the subgroup $\mathcal{R} = \{\text{id}, R, R^2\}$ of rotations by $2\pi/3$, a cyclic group of order 3. We remind the reader that $H(\vec{k})$ was defined in Fig. 2(b) and $\vec{k}^* = (2\pi/3, -2\pi/3)$.

The representations of the subgroup of symmetries \mathcal{R} are

$$(59) \quad \rho_j : R \mapsto (\tau^{-j}), \quad j = 0, 1, 2,$$

where $\tau = \exp(2\pi i/3)$. Correspondingly, the equivariant functions satisfy $R\phi(x) = \phi(M_R x) = \phi(x)\tau^{-j}$. Therefore, they have the form depicted in Fig. 13(a)-(c).

The boundary conditions of the operator $H(\vec{k}^*)$, see Fig. 2(b) with $\omega_1 = \overline{\omega_2} = \tau = \exp(2\pi i/3)$, force the choice $h_0 = \bar{\tau}f_0$, $h_1 = \tau f_1$ and $h_2 = f_2$ (it is instructive to check that this choice satisfies the boundary relations for *all pairs* of hexagon’s edges).

The functions in each isotypic component can be described uniquely by their values in one of the rhombical domains; restricting the operator $H(\vec{k}^*)$ to the lower left one, we obtain the operators Q_0 , Q_1 and Q_2 . By construction, the union (as multisets) of their spectra gives the entire spectrum of the operator $H(\vec{k}^*)$. The degeneracies in the spectrum of $H(\vec{k}^*)$ now follow from the fact that, if H had suitable additional symmetries, the operators Q_1 and Q_2 are isospectral.

We will check it using the isospectrality condition of Band, Parzanchevski and Ben-Shach, see [4, Cor. 4.4] or [30, Cor. 4].

Theorem B.3 (Band–Parzanchevski–Ben-Shach). *If \mathcal{S} acts on Γ and H_1, H_2 are subgroups of \mathcal{S} with the corresponding representations ρ_1 and ρ_2 such that the induced representations*

$$(60) \quad \text{Ind}_{H_1}^{\mathcal{S}} \rho_1 \simeq \text{Ind}_{H_2}^{\mathcal{S}} \rho_2$$

are isomorphic. Then the quotients $Q_1 = \Gamma/\rho_1$ and $Q_2 = \Gamma/\rho_2$ are isospectral.

Remark B.4. Theorem B.3 was formulated for graphs (hence the notation Γ), but it extends to manifolds with no changes when the representations ρ_j are 1- or 2-dimensional. Also, the authors did not consider the antilinear symmetries, but the extension to this case should not present any difficulties. In any case, we already have the proof of Theorem 4.1 which is a simple and constructive verification of the isospectrality of Q_1 and Q_2 in our particular setting. But we believe that checking condition (60), done in the subsections below, highlights the interesting structure of symmetry groups studied here and could be easier to extend to symmetry groups not included in our considerations.

B.2.1. R and F symmetry. Suppose the operator H on the whole space had R and F symmetry. The symmetries satisfy the relations $R^3 = F^2 = \text{id}$ and $FR^2 = RF$ and the symmetries group \mathcal{S} is thus isomorphic to the symmetric group S_3 . The representations are

$$(61) \quad R \mapsto (1), \quad F \mapsto (1) \quad \text{“trivial”},$$

$$(62) \quad R \mapsto (1), \quad F \mapsto (-1) \quad \text{“alternating”},$$

and

$$(63) \quad R \mapsto \begin{pmatrix} \tau & 0 \\ 0 & \bar{\tau} \end{pmatrix}, \quad F \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{“standard”}.$$

The subgroups H_1 and H_2 in our case are identical and given by $\mathcal{R} = \{\text{id}, R, R^2\}$. The representation $\rho_1 : R \mapsto (\tau)$, prescribes the action of the group elements of \mathcal{R} on a one-dimensional space spanned by vector \vec{v}_1 . To calculate the induced representation, we introduce the second vector $\vec{v}_2 = F\vec{v}_1$ independent of \vec{v}_1 . The action of the group generators can now be calculated as

$$(64) \quad R\vec{v}_1 = \tau\vec{v}_1, \quad F\vec{v}_1 = \vec{v}_2$$

$$(65) \quad R\vec{v}_2 = RF\vec{v}_1 = FR^2\vec{v}_1 = \bar{\tau}F\vec{v}_1 = \bar{\tau}\vec{v}_2, \quad F\vec{v}_2 = F^2\vec{v}_1 = \vec{v}_1,$$

which is precisely the standard representation of \mathcal{S} .

The representation induced by $\rho_2 : R \mapsto \bar{\tau}$ is similarly calculated to be

$$(66) \quad R\vec{v}_1 = \bar{\tau}\vec{v}_1, \quad F\vec{v}_1 = \vec{v}_2$$

$$(67) \quad R\vec{v}_2 = \tau\vec{v}_2, \quad F\vec{v}_2 = \vec{v}_1,$$

which is isomorphic to the standard representation by the change of basis $\vec{v}_1 \leftrightarrow \vec{v}_2$.

We conclude that the operators Q_1 and Q_2 are isospectral when H has reflection symmetry in addition to rotation by $2\pi/3$ and the corresponding eigenvalues of $H(\vec{k}^*)$ are (at least) doubly degenerate.

B.2.2. R and V symmetry. On the face of it, the group generated by R and V is the group of rotations by $\pi/3$, which is abelian and therefore has one-dimensional representations only. This would normally suggest there are no persistent degeneracies in the spectrum. However, the symmetry relevant to us, as explained in section 3, is V combined with complex conjugation, \bar{V} . Since the action of \bar{V} on a function ϕ is given by

$$(68) \quad (\bar{V}\phi)(x) = \overline{\phi(Vx)},$$

the definition of equivariant vectors, equation (58), has to be modified to

$$(69) \quad (\overline{\phi_1(Vx)}, \dots, \overline{\phi_n(Vx)}) = (\phi_1(x), \dots, \phi_n(x))\rho(\bar{V})^T.$$

This shows that the representation $\rho(\bar{V})$ must be an antiunitary operator — complex conjugation followed by the multiplication by a unitary matrix. Representations combining unitary and antiunitary operators have been fully classified by Wigner [41, Chap. 26] (see also [6] for a summary of the method), who called them “corepresentations”. In short, one looks at the representation of the maximal unitary subgroup (in our case, the cyclic group of rotations R) and, from them, follows a simple prescription to construct all corepresentations. This prescription is essentially constructing the induced representation *a la Frobenius*, although Wigner never identifies it as such (in one case, the induced representations decomposes into two copies of an irrep; in this case one takes only one copy).

We will now construct the induced (co)representation of the abelian group \mathcal{S} generated by R and \bar{V} . We start with the representation ρ_1 of the subgroup \mathcal{R} , see (59), acting on a 1-dimensional space spanned by \vec{v}_1 . We denote $\vec{v}_2 = \bar{V}\vec{v}_1$ and calculate

$$(70) \quad R\vec{v}_1 = \tau\vec{v}_1, \quad \bar{V}\vec{v}_1 = \vec{v}_2$$

$$(71) \quad R\vec{v}_2 = R\bar{V}\vec{v}_1 = \bar{V}R\vec{v}_1 = \bar{V}\tau\vec{v}_1 = \bar{\tau}\bar{V}\vec{v}_1 = \bar{\tau}\vec{v}_2, \quad \bar{V}\vec{v}_2 = \bar{V}^2\vec{v}_1 = \vec{v}_1.$$

The induced representation of ρ_2 is identical, after the change of basis $\vec{v}_1 \leftrightarrow \vec{v}_2$. These representations coincide with the second of the only two corepresentations of the group \mathcal{S} , given by

$$(72) \quad R : z \mapsto z, \quad \bar{V} : z \mapsto \bar{z},$$

$$(73) \quad R : \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \mapsto \begin{pmatrix} \tau z_1 \\ \bar{\tau} z_2 \end{pmatrix}, \quad \bar{V} : \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \mapsto \begin{pmatrix} \bar{z}_2 \\ \bar{z}_1 \end{pmatrix}.$$

We remark that the bars over z appear since z are scalar coefficients in the expansion over $\{\vec{v}_1, \vec{v}_2\}$ and \bar{V} is antilinear, equation (57).

B.3. R and F_V symmetry. Finally, we investigate what happens if the operator is symmetric with respect to rotation R and vertical reflection F_V , but not horizontal reflection F or inversion V .

In the dual space and k coordinates, the vertical reflection acts as the matrix

$$(74) \quad \hat{F}_V = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

and therefore preserves the line $k_2 = k_1$. The special points $\pm\vec{k}^*$ are not on this line and therefore do not benefit from the “pure” symmetry F_V . However, the vertical reflection followed by complex conjugation, denoted by \bar{F}_V preserves the line $k_1 = -k_2$ and, therefore, the special points $\pm\vec{k}^*$. The group generated by R and \bar{F}_V is S_3 , yet we should be looking at corepresentations, of which there are three, all one-dimensional,

$$(75) \quad R : z \mapsto z, \quad \bar{F}_V : z \mapsto \bar{z},$$

$$(76) \quad R : z \mapsto \tau z, \quad \bar{F}_V : z \mapsto \bar{z},$$

$$(77) \quad R : z \mapsto \bar{\tau} z, \quad \bar{F}_V : z \mapsto \bar{z}.$$

This suggests that a typical problem⁷ with these symmetries is not expected have any conical points in its dispersion relation. According to Theorem 6.1, there will still be generic degeneracies at the point $\vec{0}$ but those are not conical.

It is also easy to check that the induced representation of ρ_1 decomposes into two copies of irrep (76) and the induced representation of ρ_2 into two copies of (77).

⁷i.e. one without “accidental” degeneracies; it must be mentioned that the physically intuitive claim that “accidental” degeneracies do not happen generically remains, to a large extent, mathematically unproven; the best result in this direction is by Zelditch [44].

APPENDIX C. PERTURBATION OF PURE LAPLACIAN AND DEGENERACY AT $\vec{k} = 0$

In this section we briefly outline the situation at the quasimomentum point $\vec{k} = 0$ when the operator is $H_0 = -\Delta$. This should be compared with the discussion of Section 5.3.

The lowest eigenvalue of $H_0(0)$ is zero, its only eigenfunction is the constant function. The next eigenvalue is six-fold degenerate. The eigenfunctions are constructed out of the base function

$$(78) \quad \phi(\vec{x}) := \exp(2\pi i(\vec{b}_1 + \vec{b}_2) \cdot \vec{x}) = \exp\left(\frac{4\pi i}{\sqrt{3}}x_1\right),$$

by rotations. The symmetries of this problem are the rotation R , inversion V , reflection F and complex conjugation C . The group generated by R and V is the abelian group of rotations by $2\pi/6$, we denote this rotation by R_6 . Then the six orthogonal eigenvectors are

$$(79) \quad \psi_j(\vec{x}) := \sum_{k=0}^6 \sigma^{jk} R_6^k \phi(\vec{x}),$$

where $\sigma = \exp(2\pi i/6)$ is the principal 6-th root of unity.

The six-fold degenerate eigenspace can be decomposed into four subspaces which correspond to the irreducible representations of the group of symmetries. Namely, $\xi = \psi_0(\vec{x})$ satisfied

$$R_6 \xi = \xi, \quad F \xi = \xi, \quad C \xi = \xi,$$

eigenfunctions $\xi = \psi_1(\vec{x})$ and $\eta = -\psi_5(\vec{x})$ satisfy

$$R_6 \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} \sigma \eta \\ \sigma^5 \xi \end{pmatrix}, \quad F \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} \eta \\ \xi \end{pmatrix}, \quad C \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} \eta \\ \xi \end{pmatrix};$$

eigenfunctions $\xi = \psi_2(\vec{x})$ and $\eta = \psi_4(\vec{x})$ satisfy

$$R_6 \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} \sigma^2 \eta \\ \sigma^4 \xi \end{pmatrix}, \quad F \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} \eta \\ \xi \end{pmatrix}, \quad C \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} \eta \\ \xi \end{pmatrix};$$

finally, $\xi = i\psi_3(\vec{x})$ satisfies

$$R_6 \xi = -\xi, \quad F \xi = -\xi, \quad C \xi = \xi.$$

Perturbing the operator H_0 by a weak potential $\varepsilon q(\vec{x})$ which has all the symmetries $\{R, V, F, C\}$ will split this group of 6 eigenvalues into 4 groups corresponding to the above representations.

APPENDIX D. PERTURBATION AROUND A DEGENERATE POINT WITH F SYMMETRY

It is interesting to calculate the matrices H_1, H_2 if the degenerate eigenspace has F symmetry. Suppose the basis is chosen such that

$$F f_1 = f_1, \quad F f_2 = -f_2.$$

This can be done at the special point K if the operator has R symmetry; in section 7.2 we showed that this situation survives even if we weakly break the symmetry R .

In this case, equation (37) becomes

$$(80) \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} h_{\vec{k}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = h_{\hat{F}\vec{k}}, \quad \hat{F} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}.$$

It is easiest to evaluate $h_{\vec{k}}$ in the direction $\vec{k}_e = (1, -1)^T$, which is an eigenvector of \hat{F} with eigenvalue 1, and in the direction $\vec{k}_o = (1, 1)^T$, which is an eigenvector of \hat{F} with eigenvalue -1 . Remembering that $h_{-\vec{k}} = h_{\vec{k}}$, we get

$$(81) \quad h_{\vec{k}_e} = \begin{pmatrix} a & 0 \\ 0 & c \end{pmatrix}, \quad h_{\vec{k}_o} = \begin{pmatrix} 0 & b \\ \bar{b} & 0 \end{pmatrix},$$

In particular, the trace of the derivative matrix in the direction perpendicular to the symmetry line $k_2 = -k_1$ is zero and thus the cone can only be tilted in the direction of the symmetry line. If R symmetry is present, there is no tilt, as mentioned above.

The above picture, where the derivative matrix is diagonal in the direction preserving a symmetry, and has zeros on the diagonal in the orthogonal direction, can be generalized to other space symmetries.

Proposition D.1. *Let $H(\vec{k})$ be an operator depending on quasi-momenta \vec{k} . Assume that at point K it has a unitary \mathbb{C} -linear symmetry S whose eigenspaces we denote X_j , $j = 1, \dots$. Consider the basis of the dual \vec{k} -space, which consists of the eigenvectors of $\hat{S} = S^*$. If the vector \vec{e} corresponds to eigenvalue 1 then*

$$\partial_{\vec{e}} H X_j \subset X_j, \quad \text{for all } j.$$

If the vector \vec{k} corresponds to eigenvalue other than 1 then

$$\partial_{\vec{e}} H X_j \perp X_j, \quad \text{for all } j.$$

APPENDIX E. BERRY PHASE AROUND A CONICAL POINT

Here, for completeness, we give a proof of the fact that the Berry phase around a nondegenerate conical point is π , which has been formulated as Lemma 7.1. The proof is geometrical in nature and avoids the direct computation used in the original articles [19, 5].

Presence of the antiunitary symmetry \bar{V} which squares to -1 allows us to choose special bases for eigenspaces. We will be using the following lemma.

Lemma E.1. *Let A be an antiunitary involution on a separable Hilbert space X . Then*

(1) *there is an orthonormal basis $\{f_j\}$ of vectors such that*

$$(82) \quad Af_j = f_j.$$

(2) *if $\dim(X) = 2$, there exists a basis $\{\psi, A\psi\}$.*

Proof. To prove the first part, we start with an arbitrary basis $\{\psi_j\}$. Then the vectors

$$f_j^+ = \psi_j + A\psi_j, \quad \text{and} \quad f_j^- = i(\psi_j - A\psi_j)$$

both satisfy $Af = f$ and have the vector ψ_j in their span. Therefore, the set $\{f_j^+, f_j^-\}$ spans the whole space and can be made into a orthonormal basis by applying the Gram-Schmidt process. This preserves property (82) since all coefficients arising in the process are real:

$$\langle f, f' \rangle = \langle Af, Af' \rangle = \overline{\langle f, f' \rangle} \in \mathbb{R}.$$

To get the second part from the first we start with the orthonormal basis $\{f_1, f_2\}$ satisfying (82) and then take

$$\psi = (f_1 + if_2)/\sqrt{2}, \quad A\psi = (f_1 - if_2)/\sqrt{2},$$

which can be checked to be orthonormal. □

Now we are in the position to prove Lemma 7.1.

Proof of Lemma 7.1. Representing the parameters around the location of the conical point in polar form we will study the limiting eigenvectors

$$(83) \quad \psi_0^\pm(\theta) = \lim_{r \rightarrow 0} \psi^\pm(r, \theta),$$

where ψ^- and ψ^+ are the eigenvectors of the lower and upper branches of the cone, correspondingly. We normalize these eigenvectors and fix the phase to have

$$(84) \quad \bar{V}\psi^\pm = \psi^\pm.$$

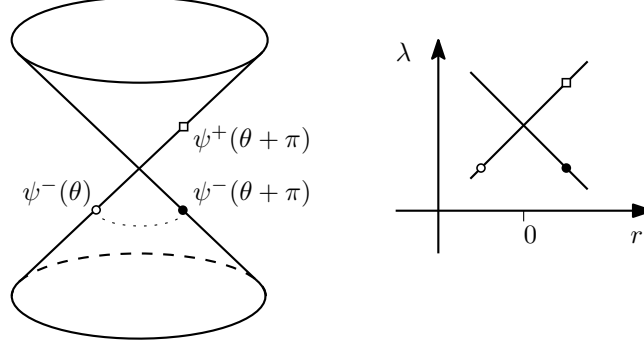


FIGURE 14. Cone with a schematic representation of a circular contour (left); a cross-section of the cone by a plane through λ axis in the direction ϕ (right).

Because the cone is nondegenerate (and thus $|\lambda_1^+(\theta) - \lambda_1^-(\theta)| > 0$), the limit exists and is continuous in θ , see equation (29).

The functions $\psi_0^\pm(\theta)$ have a curious property: since the section of the cone by a vertical plane is two intersecting lines, Fig. 14, the vector $\psi_0^+(\theta + \pi)$ is the same as $s_1\psi_0^-(\theta)$, where $s_1 = \pm 1$.

We expand ψ_0^\pm in a fixed basis of eigenvectors at the conical point, which we can choose to be of the form $\{\phi, \bar{V}\phi\}$,

$$\psi_0^\pm = \alpha^\pm(\theta)\phi + \beta^\pm(\theta)\bar{V}\phi.$$

From condition (84) we immediately get $\beta^\pm = \overline{\alpha^\pm}$. On the other hand, the vectors ψ_0^+ and ψ_0^- are orthogonal, leading to the condition

$$\overline{\alpha^+}\alpha^- + \alpha^+\overline{\alpha^-} = 0 \quad \text{or} \quad \overline{\alpha^+}\alpha^- \in i\mathbb{R}.$$

From normalization of ψ_0^\pm , we conclude that $\alpha^- = i\alpha^+s_2$, where $s_2 = \pm 1$. We therefore get

$$\alpha^+(\theta + \pi) = \alpha^-(\theta)s_1 = i\alpha^+(\theta)s_1s_2,$$

and, therefore,

$$\alpha^+(\theta + 2\pi) = (is_1s_2)^2\alpha^+(\theta) = -\alpha^+(\theta).$$

□

We remark that in the proof above, the overall sign s_1s_2 determines the direction of rotation of the vectors $\psi_0^\pm(\theta)$ in the two-dimensional space.

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REFERENCES

- [1] V. I. Arnold. *Mathematical methods of classical mechanics*, volume 60 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, second edition, 1989. Translated from the 1974 Russian original by K. Vogtmann and A. Weinstein.
- [2] J. E. Avron and B. Simon. Analytic properties of band functions. *Ann. Physics*, 110(1):85–101, 1978.
- [3] O. Bahat-Treidel, O. Peleg, and M. Segev. Symmetry breaking in honeycomb photonic lattices. *Opt. Lett.*, 33(19):2251–2253, 2008.
- [4] R. Band, O. Parzanchevski, and G. Ben-Shach. The isospectral fruits of representation theory: quantum graphs and drums. *J. Phys. A*, 42(17):175202, 42, 2009.
- [5] M. V. Berry. Quantal phase factors accompanying adiabatic changes. *Proc. Roy. Soc. London Ser. A*, 392(1802):45–57, 1984.
- [6] C. J. Bradley and B. L. Davies. Magnetic groups and their corepresentations. *Rev. Modern Phys.*, 40:359–379, 1968.
- [7] P. Buser, J. Conway, P. Doyle, and K.-D. Semmler. Some planar isospectral domains. *Internat. Math. Res. Notices*, (9):391–400, 1994.
- [8] A. Castro Neto, F. Guinea, N. Peres, K. Novoselov, and A. Geim. The electronic properties of graphene. *Rev. Mod. Phys.*, 81:109–162, 2009.
- [9] N. T. Do and P. Kuchment. Quantum graph spectra of a graphyne structure. *Nanoscale Systems: Mathematical Modeling, Theory and Applications*, 2:107–123, 2013.
- [10] P. Exner, P. Kuchment, and B. Winn. On the location of spectral edges in \mathbb{Z} -periodic media. *J. Phys. A*, 43(47):474022, 8, 2010.
- [11] C. L. Fefferman, J. P. Lee-Thorp, and M. I. Weinstein. Topologically protected states in one-dimensional systems. preprint [arXiv:1405.4569 \[math-ph\]](https://arxiv.org/abs/1405.4569), 2014.
- [12] C. L. Fefferman and M. I. Weinstein. Honeycomb lattice potentials and Dirac points. *J. Amer. Math. Soc.*, 25(4):1169–1220, 2012.
- [13] C. L. Fefferman and M. I. Weinstein. Wave packets in honeycomb structures and two-dimensional Dirac equations. *Comm. Math. Phys.*, 326(1):251–286, 2014.
- [14] M. Golubitsky, I. Stewart, and D. G. Schaeffer. *Singularities and groups in bifurcation theory. Vol. II*, volume 69 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1988.
- [15] R. Goodman and N. R. Wallach. *Symmetry, Representations, and Invariants*, volume 255 of *Graduate Texts in Mathematics*. Springer New York, 2009.
- [16] C. Gordon, D. Webb, and S. Wolpert. Isospectral plane domains and surfaces via Riemannian orbifolds. *Invent. Math.*, 110(1):1–22, 1992.
- [17] V. Grushin. Multiparameter perturbation theory of Fredholm operators applied to Bloch functions. *Math. Notes*, 86(5-6):767–774, 2009.
- [18] J. M. Harrison, P. Kuchment, A. Sobolev, and B. Winn. On occurrence of spectral edges for periodic operators inside the Brillouin zone. *J. Phys. A*, 40(27):7597–7618, 2007.
- [19] G. Herzberg and H. C. Longuet-Higgins. Intersection of potential energy surfaces in polyatomic molecules. *Discuss. Faraday Soc.*, 35:77–82, 1963.
- [20] T. Kato. *Perturbation theory for linear operators*. Springer-Verlag, Berlin, second edition, 1976. Grundlehren der Mathematischen Wissenschaften, Band 132.
- [21] M. I. Katsnelson. *Graphene: Carbon in Two Dimensions*. Cambridge University Press, 2012.
- [22] P. Kuchment. *Floquet theory for partial differential equations*, volume 60 of *Operator Theory: Advances and Applications*. Birkhäuser Verlag, Basel, 1993.
- [23] P. Kuchment and O. Post. On the spectra of carbon nano-structures. *Comm. Math. Phys.*, 275(3):805–826, 2007.
- [24] A. Luican, G. Li, A. Reina, J. Kong, R. R. Nair, K. S. Novoselov, A. K. Geim, and E. Y. Andrei. Single-layer behavior and its breakdown in twisted graphene layers. *Phys. Rev. Lett.*, 106:126802, Mar 2011.
- [25] J. L. Mañes. Existence of bulk chiral fermions and crystal symmetry. *Phys. Rev. B*, 85:155118, 2012.
- [26] J. L. Mañes, F. Guinea, and M. A. H. Vozmediano. Existence and topological stability of fermi points in multi-layered graphene. *Phys. Rev. B*, 75:155424, 2007.
- [27] D. Monaco and G. Panati. Topological invariants of eigenvalue intersections and decrease of Wannier functions in graphene. *J. Stat. Phys.*, 155(6):1027–1071, 2014.
- [28] K. Novoselov. Nobel lecture: Graphene: Materials in the flatland. *Rev. Mod. Phys.*, 83:837–849, 2011.
- [29] K. R. Parthasarathy. Projective unitary antiunitary representations of locally compact groups. *Comm. Math. Phys.*, 15:305–328, 1969.
- [30] O. Parzanchevski and R. Band. Linear representations and isospectrality with boundary conditions. *J. Geom. Anal.*, 20(2):439–471, 2010.

- [31] L. A. Ponomarenko, R. V. Gorbachev, G. L. Yu, D. C. Elias, R. Jalil, A. A. Patel, A. Mishchenko, A. S. Mayorov, C. R. Woods, J. R. Wallbank, M. Mucha-Kruczynski, B. A. Piot, M. Potemski, I. V. Grigorieva, K. S. Novoselov, F. Guinea, V. I. Fal'ko, and A. K. Geim. Cloning of Dirac fermions in graphene superlattices. *Nature*, 497(7451):594–597, 2013.
- [32] F. Rellich. Störungstheorie der Spektralzerlegung, III. *Math. Ann.*, 116(1):555–570, 1939.
- [33] B. Simon. Holonomy, the quantum adiabatic theorem, and Berry's phase. *Phys. Rev. Lett.*, 51(24):2167–2170, 1983.
- [34] J. C. Slonczewski and P. R. Weiss. Band structure of graphite. *Phys. Rev.*, 109(2):272–279, 1958.
- [35] T. Sunada. Riemannian coverings and isospectral manifolds. *Ann. of Math. (2)*, 121(1):169–186, 1985.
- [36] L. Tarruell, D. Greif, T. Uehlinger, G. Jotzu, and T. Esslinger. Creating, moving and merging Dirac points with a Fermi gas in a tunable honeycomb lattice. *Nature*, 483(7389):302–305, 2012.
- [37] P. R. Wallace. The band theory of graphite. *Phys. Rev.*, 71:622–634, May 1947.
- [38] J. R. Wallbank, A. A. Patel, M. Mucha-Kruczyński, A. K. Geim, and V. I. Fal'ko. Generic miniband structure of graphene on a hexagonal substrate. *Phys. Rev. B*, 87:245408, 2013.
- [39] J. Weidmann. *Linear operators in Hilbert spaces*, volume 68 of *Graduate Texts in Mathematics*. Springer-Verlag, New York-Berlin, 1980.
- [40] H. Weyl. *The Classical Groups. Their Invariants and Representations*. Princeton University Press, Princeton, N.J., 1939.
- [41] E. P. Wigner. *Group theory and its applications to the quantum mechanics of atomic spectra*. Academic Press, New York, 1959.
- [42] M. Yankowitz, J. Xue, D. Cormode, J. D. Sanchez-Yamagishi, K. Watanabe, T. Taniguchi, P. Jarillo-Herrero, P. Jacquod, and B. J. LeRoy. Emergence of superlattice Dirac points in graphene on hexagonal boron nitride. *Nat. Phys.*, 8:382–386, 2012.
- [43] M. G. Zaidenberg, S. Krein, P. A. Kuchment, and A. A. Pankov. Banach bundles and linear operators. *Russian Math. Surveys*, 30(5):115, 1975.
- [44] S. Zelditch. On the generic spectrum of a Riemannian cover. *Ann. Inst. Fourier (Grenoble)*, 40(2):407–442, 1990.

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